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TI	Title of Document
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URL	Uniform Resource Locator
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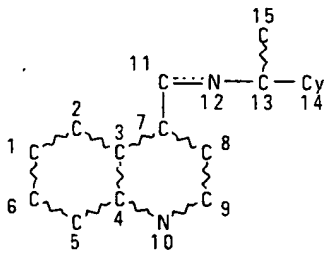
DS	Designated States (patent)
AI	Patent Application Information
PRAI	Priority Application Information
DT	Document Type
PY	Publication Year
LA	Language
IC	International Patent Classification (IPC)
ICM	Main IPC
ICS	Secondary IPC
ICA	Additional or Supplementary IPC
ICI	Index or Complementary IPC
NCL	National Patent Classification Code
CC	Classification Code (CA Section Code and Title and CA Section Cross-Reference Code)

OS	Other Source
GI	Graphic Image
AB	Abstract
ST	Supplementary Term (CA Keywords)
IT	Index Term

17 ANSWERS PRINTED IN FORMAT 'BIB ABS HITSTR'
IN FILE 'CA'
USING QUERY:
L1 STR



NODE ATTRIBUTES:
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DEFAULT MLEVEL IS ATOM
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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L2 220 SEA FILE=REGISTRY SSS FUL L1
L3 17 SEA FILE=CA L2
L4 17 SEA FILE=CAPLUS L2
L5 34 SEA L2
L6 17 DUP REM L5 (17 DUPLICATES REMOVED)

L6 ANSWER 1 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 1

AN 127:121650 CA

TI Preparation of quinoline-4-carboxamides as NK-2/NK-3 antagonists

IN Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farino, Carlo

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farino, Carlo

SO PCT Int. Appl., 61 pp.
CODEN: PIXXD2

PI WO 9721680 A1 970619

DS TT, W UA, W UG, W US, W UZ, W VN, W AM, W AZ, W BY, W KG, W KZ, W MD, W RU, W TJ, W TM, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 96-EP5203 961122

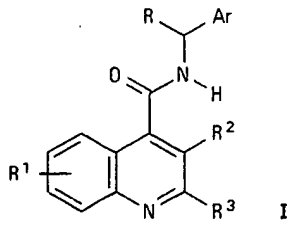
PRAI IT 95-MI2461 951124
IT 96-MI1689 960802

DT Patent

LA English

OS MARPAT 127:121650

GI



I

AB The title compds. [I; Ar = (un)substituted aryl, C_{5-7} cycloalkadienyl (un)substituted heteroaryl; R = C_{1-6} alkyl, C_{3-7} cycloalkyl, (un)substituted Ph; R^1 = H, C_{1-6} alkyl, aryl, etc.; R^2 = $O(CH_2)_nX$ (wherein X = (un)substituted alkyl, NH_2, etc.), etc.; R^3 = C_{1-6} alkyl, C_{3-7} cycloalkyl, (un)substituted aryl], useful for the treatment and/or prophylaxis of respiratory diseases in mammals, were prepd. Thus, reaction of (S)-N-(α-ethylbenzyl)-3-hydroxy-2-phenylquinoline-4-carboxamide with Et bromoacetate in the presence of K_2CO_3 and KI in THF followed by hydrolysis with 37% HCl afforded (S)-I.HCl [Ar = Ph; R = Et; R^1 = H; R^2 = OCH_2COOH; R^3 = Ph] which showed IC_{50} of 1.9 nM

L6 ANSWER 1 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 1

against human neurokinin-3 receptors binding in CHO cell lines.

IT ***191796-72-2P*** ***192704-65-7P*** ***192704-72-6P*** ***192704-73-7P***

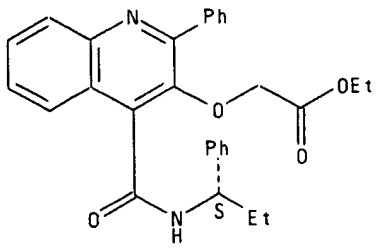
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinoline-4-carboxamides as NK-2/NK-3 antagonists)

RN 191796-72-2 CA

CN Acetic acid, [[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, ethyl ester, (*S*)- (9CI) (CA INDEX NAME)

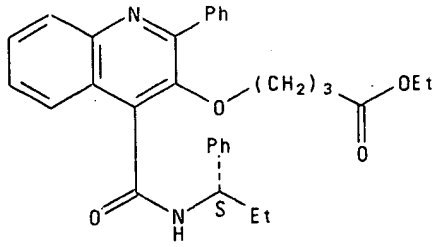
Absolute stereochemistry. Rotation (-).



RN 192704-65-7 CA

CN Butanoic acid, 4-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, ethyl ester, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

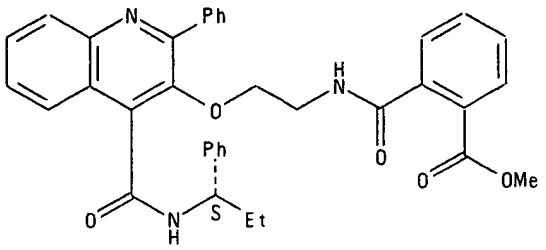


RN 192704-72-6 CA

CN Benzoic acid, 2-[[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]carbonyl]-, methyl ester, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-72-6 CA

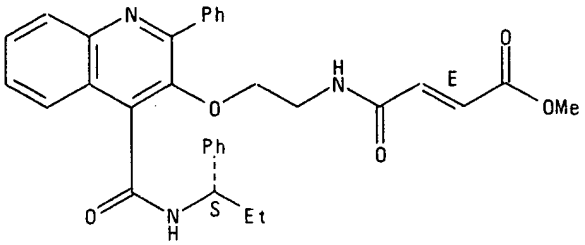


RN 192704-73-7 CA

CN 2-Butenoic acid, 4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, methyl ester, [*S*-(*E*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



IT ***191796-68-6P*** ***191796-69-7P*** ***191796-70-0P*** ***191796-77-7P*** ***191796-78-8P*** ***191796-79-9P*** ***191796-80-2P*** ***191796-81-3P*** ***191796-82-4P*** ***192704-51-1P*** ***192704-53-3P*** ***192704-55-5P*** ***192704-57-7P*** ***192704-59-9P*** ***192704-60-2P*** ***192704-61-3P*** ***192704-63-5P*** ***192704-67-9P*** ***192704-71-5P*** ***192704-75-9P*** ***192704-77-1P*** ***192704-78-2P*** ***192704-80-6P*** ***192704-86-2P*** ***192704-87-3P*** ***192704-89-5P*** ***192704-91-9P*** ***192704-92-0P*** ***192704-93-1P*** ***192704-94-2P*** ***192704-95-3P*** ***192704-97-5P*** ***192704-99-7P*** ***192705-01-4P*** ***192705-02-5P*** ***192705-04-7P*** ***192705-06-9P*** ***192705-08-1P*** ***192816-63-0P*** ***192816-65-2P*** ***192816-67-4P*** ***192816-68-5P*** ***192816-69-6P***

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

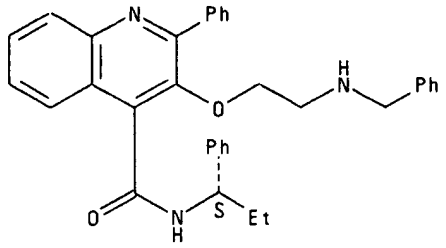
(prepn. of quinoline-4-carboxamides as NK-2/NK-3 antagonists)

RN 191796-68-6 CA

RN 191796-68-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(phenylmethyl)amino]ethoxy]-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

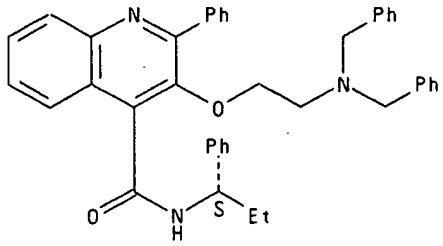


• HCl

RN 191796-69-7 CA

CN 4-Quinolinecarboxamide, 3-[2-[bis(phenylmethyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



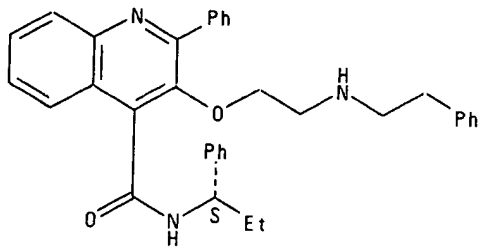
• HCl

RN 191796-70-0 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(2-phenylethyl)amino]ethoxy]-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-70-0 CA

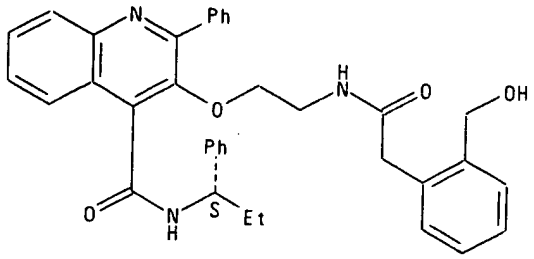


• HCl

RN 191796-77-7 CA

CN 4-Quinolinecarboxamide, 3-[2-[[[2-(hydroxymethyl)phenyl]acetyl]amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

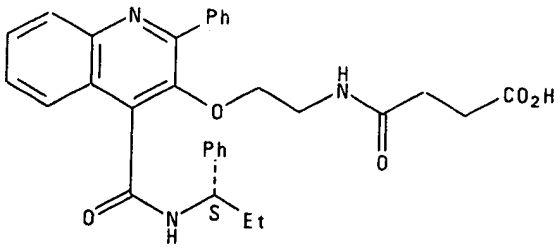
Absolute stereochemistry. Rotation (-).



RN 191796-78-8 CA

CN Butanoic acid, 4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



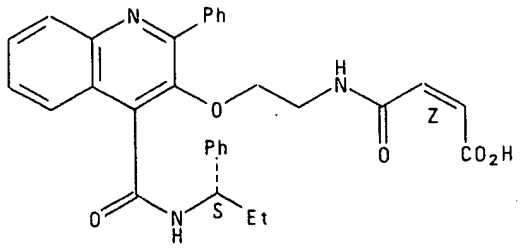
RN 191796-79-9 CA

RN 191796-79-9 CA

CN 2-Butenoic acid, 4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, [*S*-(*Z*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

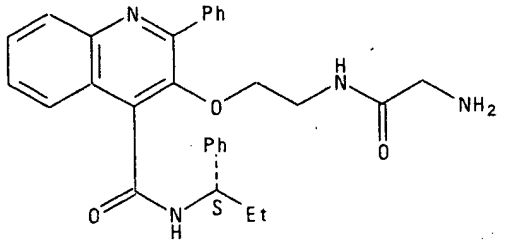
Double bond geometry as shown.



RN 191796-80-2 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminoacetyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

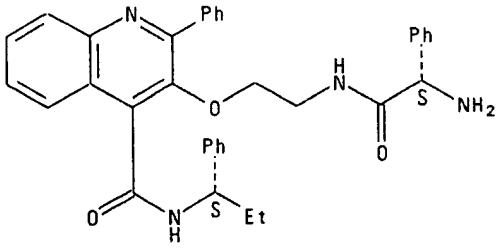
Absolute stereochemistry. Rotation (-).



RN 191796-81-3 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [*S*-(*R**,*R**)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

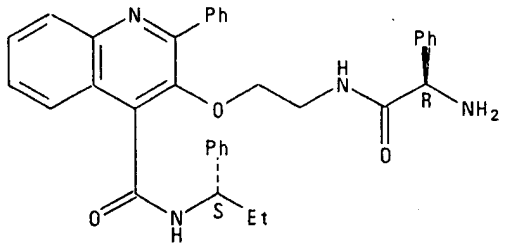


RN 191796-82-4 CA

RN 191796-82-4 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [*S*-(*R**,*S**)]- (9CI) (CA INDEX NAME)

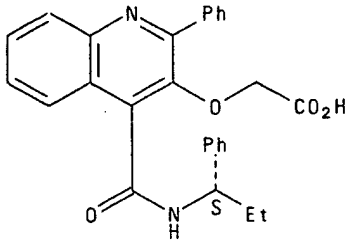
Absolute stereochemistry. Rotation (-).



RN 192704-51-1 CA

CN Acetic acid, [[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

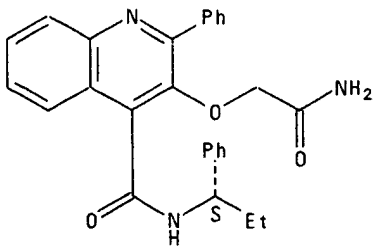


• HCl

RN 192704-53-3 CA

CN 4-Quinolinecarboxamide, 3-(2-amino-2-oxoethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

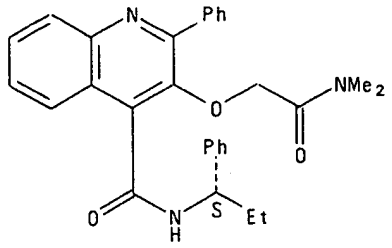


RN 192704-53-3 CA

RN 192704-55-5 CA

CN 4-Quinolinecarboxamide, 3-[2-(dimethylamino)-2-oxoethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

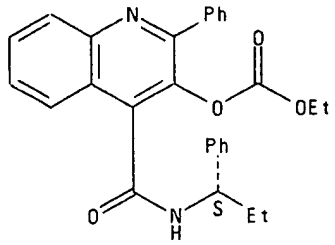
Absolute stereochemistry. Rotation (-).



RN 192704-57-7 CA

CN Carbonic acid, ethyl 2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl ester, (*S*)- (9CI) (CA INDEX NAME)

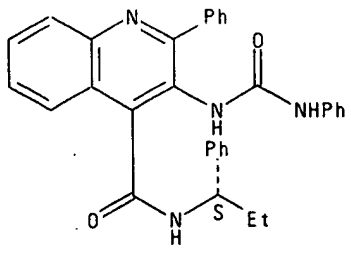
Absolute stereochemistry. Rotation (-).



RN 192704-59-9 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[[(phenylamino)carbonyl]amino]-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

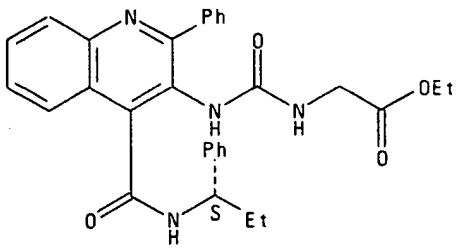


RN 192704-60-2 CA

RN 192704-60-2 CA

CN Glycine, *N*-[[[2-phenyl-4-[[[(1*S*)-1-phenylpropyl]amino]carbonyl]-3-quinolinyl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

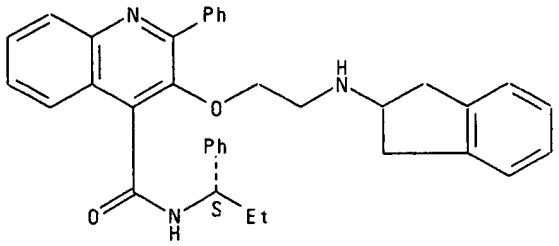
Absolute stereochemistry. Rotation (-).



RN 192704-61-3 CA

CN 4-Quinolinecarboxamide, 3-[2-[(2,3-dihydro-1*H*-inden-2-yl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

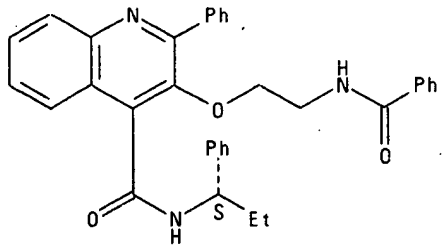


• HCl

RN 192704-63-5 CA

CN 4-Quinolinecarboxamide, 3-[2-(benzoylamino)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

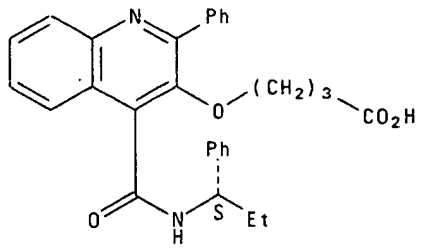


RN 192704-63-5 CA

RN 192704-67-9 CA

CN Butanoic acid, 4-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, (*S*)- (9CI) (CA INDEX NAME)

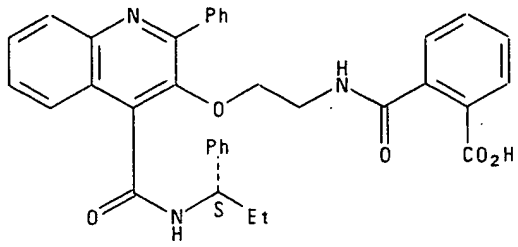
Absolute stereochemistry. Rotation (-).



RN 192704-71-5 CA

CN Benzoic acid, 2-[[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]carbonyl]-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



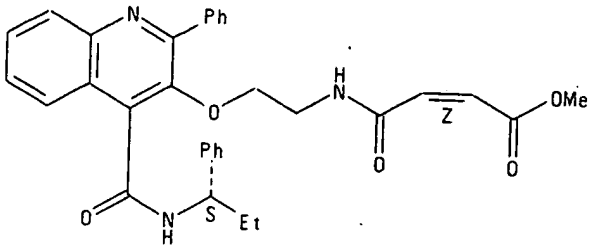
RN 192704-75-9 CA

CN 2-Butenoic acid, 4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, methyl ester, [*S*-(*Z*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

RN 192704-75-9 CA

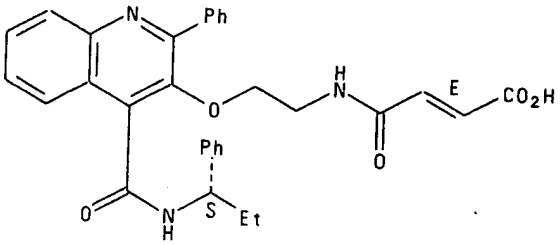


RN 192704-77-1 CA

CN 2-Butenoic acid, 4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, [*S*-(*E*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

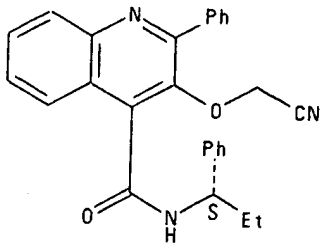
Double bond geometry as shown.



RN 192704-78-2 CA

CN 4-Quinolinecarboxamide, 3-(cyanomethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

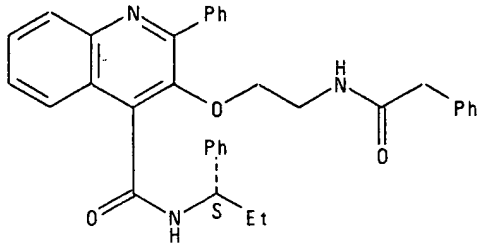


RN 192704-80-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(phenylacetyl)amino]ethoxy]-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

RN 192704-80-6 CA

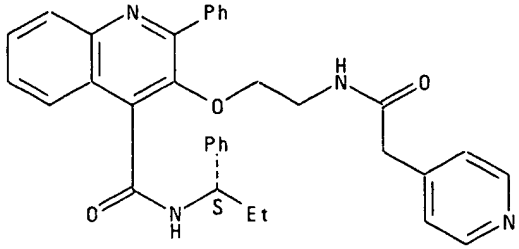
Absolute stereochemistry. Rotation (-).



RN 192704-86-2 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-[(4-pyridinylacetyl)amino]ethoxy]-, (*S*)- (9CI) (CA INDEX NAME)

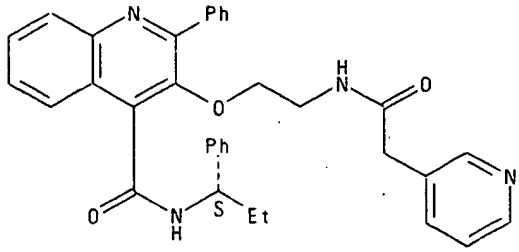
Absolute stereochemistry. Rotation (-).



RN 192704-87-3 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-[(3-pyridinylacetyl)amino]ethoxy]-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

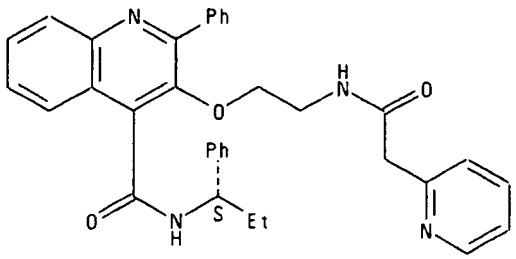


RN 192704-89-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-[(2-pyridinylacetyl)amino]ethoxy]-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

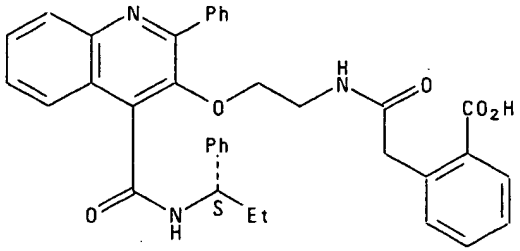
RN 192704-89-5 CA



RN 192704-91-9 CA

CN Benzoic acid, 2-[2-oxo-2-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]ethyl]-, (*S*)- (9CI) (CA INDEX NAME)

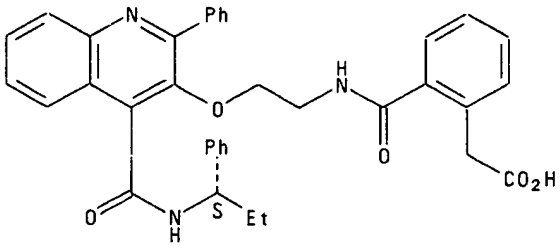
Absolute stereochemistry. Rotation (-).



RN 192704-92-0 CA

CN Benzeneacetic acid, 2-[[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]carbonyl]-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

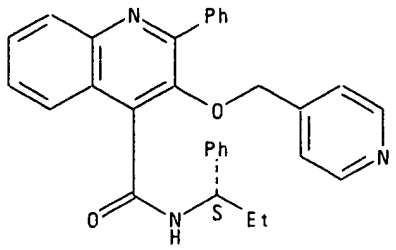


RN 192704-93-1 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-(4-pyridinylmethoxy)-, (*S*)- (9CI) (CA INDEX NAME)

RN 192704-93-1 CA

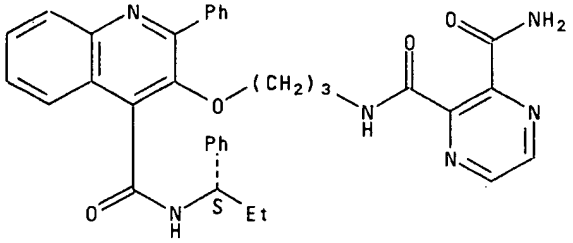
Absolute stereochemistry.



RN 192704-94-2 CA

CN 2,3-Pyrazinedicarboxamide, *N*-[3-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]propyl]-, (*S*)- (9CI) (CA INDEX NAME)

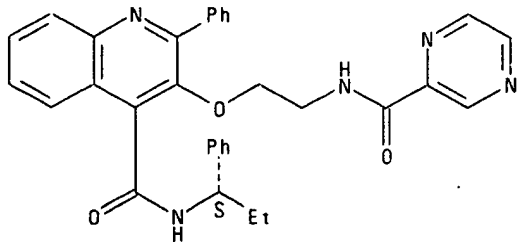
Absolute stereochemistry.



RN 192704-95-3 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-[(pyrazinylcarbonyl)amino]ethoxy]-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

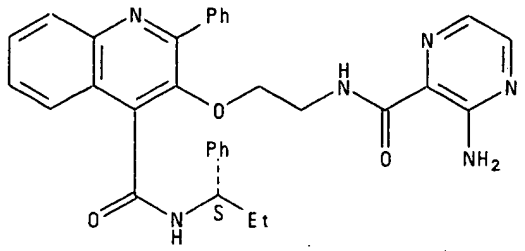


RN 192704-97-5 CA

CN 4-Quinolinecarboxamide, 3-[2-[[(3-aminopyrazinyl)carbonyl]amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

RN 192704-97-5 CA

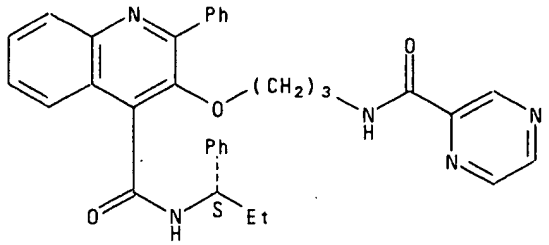
Absolute stereochemistry.



RN 192704-99-7 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[3-[(pyrazinylcarbonyl)amino]propoxy]-, (*S*)- (9CI) (CA INDEX NAME)

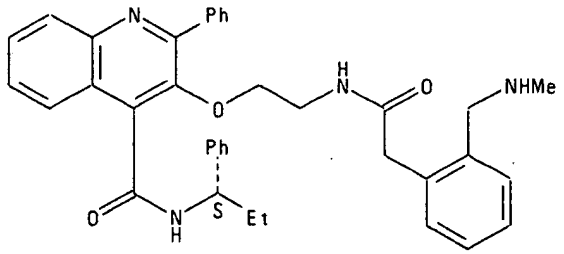
Absolute stereochemistry.



RN 192705-01-4 CA

CN 4-Quinolinecarboxamide, 3-[2-[[[2-[(methylamino)methyl]phenyl]acetyl]amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

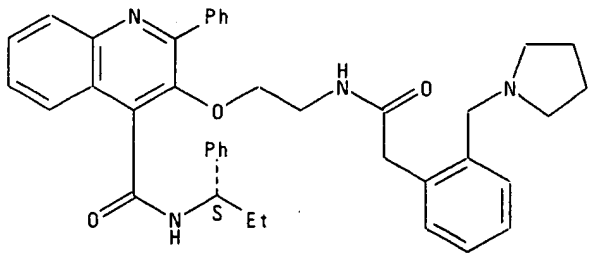


RN 192705-02-5 CA

RN 192705-02-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-[[[2-(1-pyrrolidinylmethyl)phenyl]acetyl]amino]ethoxy]-, (*S*)- (9CI) (CA INDEX NAME)

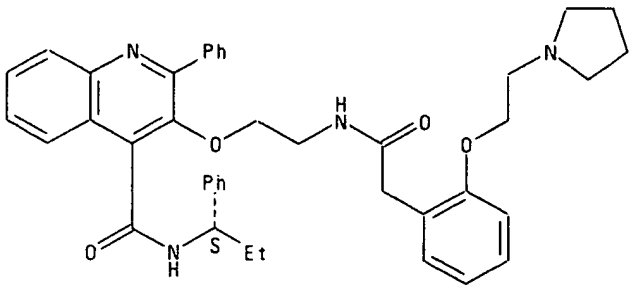
Absolute stereochemistry.



RN 192705-04-7 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-[[[2-[2-(1-pyrrolidinyl)ethoxy]phenyl]acetyl]amino]ethoxy]-, (*S*)- (9CI) (CA INDEX NAME)

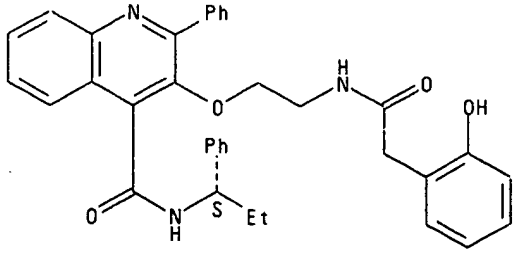
Absolute stereochemistry.



RN 192705-06-9 CA

CN 4-Quinolinecarboxamide, 3-[2-[[(2-hydroxyphenyl)acetyl]amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

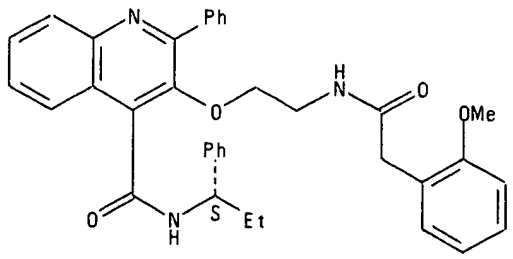


RN 192705-06-9 CA

RN 192705-08-1 CA

CN 4-Quinolinecarboxamide, 3-[2-[[(2-methoxyphenyl)acetyl]amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

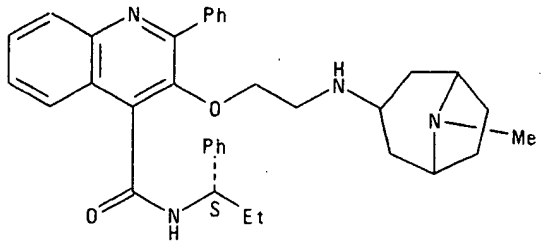
Absolute stereochemistry.



RN 192816-63-0 CA

CN 4-Quinolinecarboxamide, 3-[2-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.



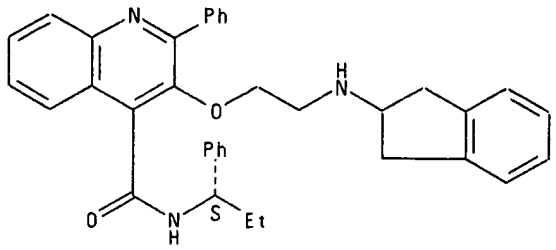
• HCl

RN 192816-65-2 CA

CN 4-Quinolinecarboxamide, 3-[2-[(2,3-dihydro-1*H*-inden-2-yl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

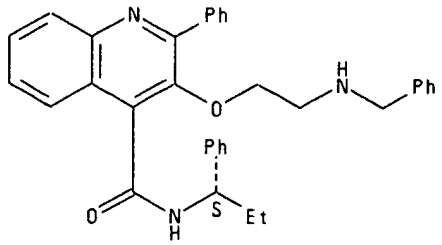
RN 192816-65-2 CA



RN 192816-67-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(phenylmethyl)amino]ethoxy]-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

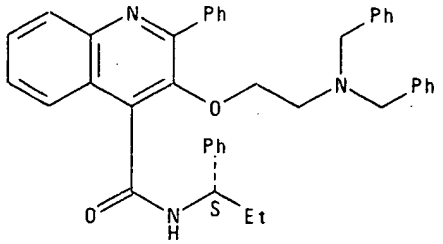
Absolute stereochemistry. Rotation (-).



RN 192816-68-5 CA

CN 4-Quinolinecarboxamide, 3-[2-[bis(phenylmethyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

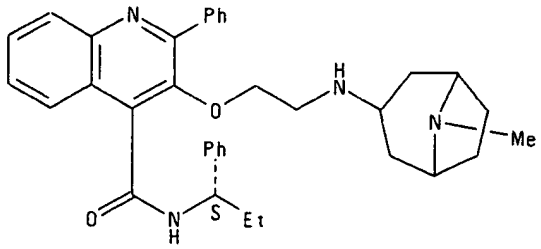


RN 192816-69-6 CA

CN 4-Quinolinecarboxamide, 3-[2-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192816-69-6 CA



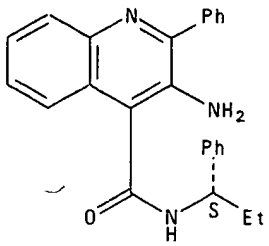
IT ***174636-16-9P*** ***174636-32-9P*** ***191796-73-3P*** ***191796-74-4P*** ***192705-11-6P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of quinoline-4-carboxamides as NK-2/NK-3 antagonists)

RN 174636-16-9 CA

CN 4-Quinolinecarboxamide, 3-amino-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

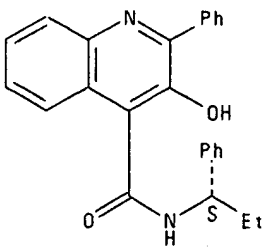
Absolute stereochemistry. Rotation (-).



RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

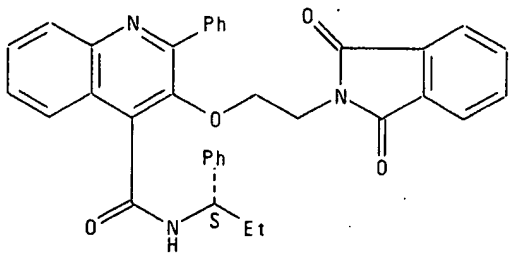


RN 191796-73-3 CA

RN 191796-73-3 CA

CN 4-Quinolinecarboxamide, 3-[2-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

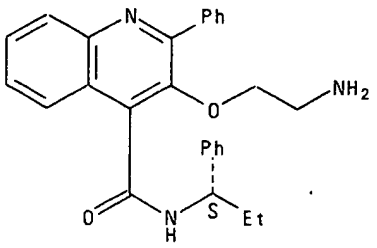
Absolute stereochemistry. Rotation (-).



RN 191796-74-4 CA

CN 4-Quinolinecarboxamide, 3-(2-aminoethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

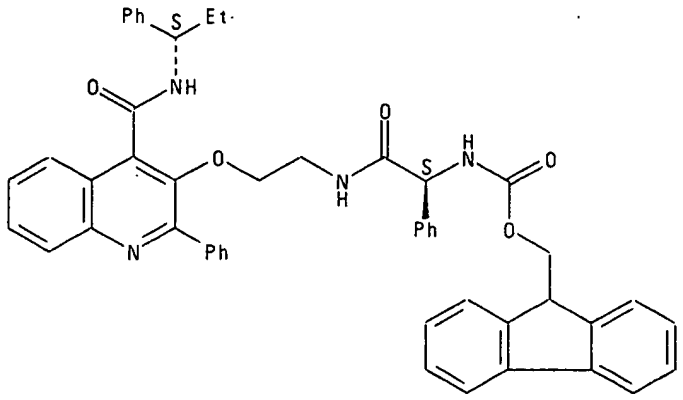


RN 192705-11-6 CA

CN Carbamic acid, [2-oxo-1-phenyl-2-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-ethyl]-, 9*H*-fluoren-9-ylmethyl ester, [*S*-(*R**,*R**)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192705-11-6 CA



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L6 ANSWER 2 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 2

AN 127:81363 CA

TI Preparation of 4-quinolinecarboxamide salt derivatives as neurokinin-3 receptor antagonists

IN Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2

PI WO 9719928 A1 970605

DS TT, W UA, W UG, W US, W UZ, W VN, W AM, W AZ, W BY, W KG, W KZ, W MD, W RU, W TJ, W TM, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 96-EP5210 961122

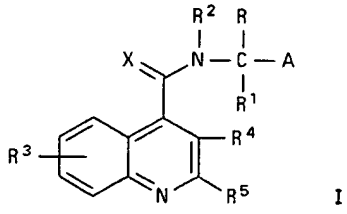
PRAI GB 95-24137 951124

DT Patent

LA English

OS MARPAT 127:81363

GI



I

AB The title salt compds. [I; A = (un)substituted Ph, (un)substituted naphthyl, (un)substituted C_{5-7} cycloalkadienyl, (un)substituted single or fused-ring heterocyclyl; R = C_{1-8} alkyl, cycloalkyl, (un)substituted Ph, (un)substituted 5-member heterocyclyl, etc.; R^1, R^2 = H, alkyl; R^3, R^4 = H, alkyl, alkenyl, aryl, alkoxy, OH, halogen, NO_2, CN, (un)substituted NH_2, etc.; R^5 = alkyl, cycloalkyl, (un)substituted aryl, etc.; X = O, S, NC:N], useful as neurokinin-3 receptor antagonists, are prepd. Thus, (S)-(-)-N-(α-ethylbenzyl)-3-hydroxy-2-phenyl-4-quinolinecarboxamide was dissolved in aq. MeOH contg. NaOH and heated to 40°, producing (S)-(+)-N-(α-ethylbenzyl)-3-hydroxy-2-phenyl-4-quinolinecarboxamide sodium salt sesquihydrate, m.p. 110° (decompn.), which demonstrated a K_i of 4.8 nM for the displacement of [^{3}H]-senktide from guinea pig cortex membrane-derived NK_3 receptors.

IT ***191786-18-2P***

L6 ANSWER 2 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 2

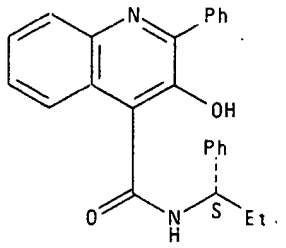
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 4-quinolinecarboxamide salt derivs. as neurokinin-3 receptor antagonists)

RN 191786-18-2 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, monosodium salt, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



• Na

IT ***174636-32-9P***

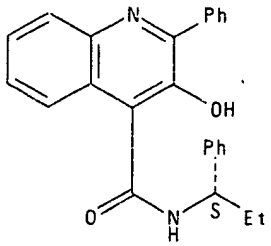
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of 4-quinolinecarboxamide salt derivs. as neurokinin-3 receptor antagonists)

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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L6 ANSWER 3 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 3

AN 127:95205 CA

TI Preparation of quinoline-derivative NK_3 receptor antagonists

IN Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

SO PCT Int. Appl., 101 pp.
CODEN: PIXXD2

PI WO 9719927 A1 970605

DS W: JP, US
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AI WO 96-EP5209 961122

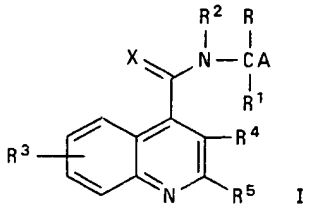
PRAI GB 95-24104 951124

DT Patent

LA English

OS MARPAT 127:95205

GI



I

AB The title compds. [I; A = (un)substituted Ph, (un)substituted naphthyl, C_{5-7} cycloalkdienyl, (un)substituted heterocyclyl; R = C_{1-8} alkyl, C_{3-7} cycloalkyl, C_{4-7} cycloalkylalkyl, (un)substituted Ph, phenylalkyl, etc.; R^1, R^2 = H, C_{1-6} alkyl, or together form a $(CH_2)_n$, etc.; n = 3-5; R^3, R^4 = H, C_{1-6} alkyl, C_{1-6} alkenyl, aryl, C_{1-6} alkoxy, hydroxy, halogen, nitro, cyano, carboxy, carboxamido, sulfonamido, C_{1-6} alkoxycarbony, trifluoromethyl, acyloxy, phthalimido, (un)substituted amino, etc.; R^5 = C_{1-6} alkyl, C_{3-7} cycloalkyl, etc.; X = O, S, NC:N; etc.], which are NK_3 receptor antagonists (no data), are prepd. Thus, α-methylbenzylamine was amidated with 2-phenylquinoline-4-carbonyl chloride, producing N-(α-methylbenzyl)-2-phenyl-4-quinolinecarboxamide, m.p. 156-157°.

IT ***174635-48-4P*** ***174635-49-5P*** ***174635-50-8P*** ***174635-51-9P*** ***174635-52-0P*** ***174635-53-1P*** ***174635-54-2P*** ***174635-55-3P*** ***174635-56-4P*** ***174635-57-5P*** ***174635-58-6P*** ***174635-59-7P*** ***174635-60-0P*** ***174635-61-1P*** ***174635-62-2P*** ***174635-63-3P*** ***174635-64-4P*** ***174635-65-5P*** ***174635-66-6P*** ***174635-68-8P*** ***174635-69-9P***

L6 ANSWER 3 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 3

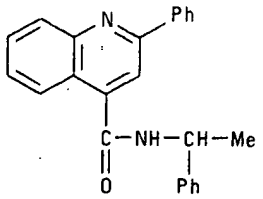
174635-70-2P ***174635-71-3P*** ***174635-72-4P*** ***174635-73-5P*** ***174635-74-6P*** ***174635-75-7P*** ***174635-76-8P*** ***174635-77-9P*** ***174635-78-0P*** ***174635-79-1P*** ***174635-80-4P*** ***174635-81-5P*** ***174635-82-6P*** ***174635-83-7P*** ***174635-84-8P*** ***174635-85-9P*** ***174635-86-0P*** ***174635-87-1P*** ***174635-88-2P*** ***174635-89-3P*** ***174635-90-6P*** ***174635-91-7P*** ***174635-92-8P*** ***174635-93-9P*** ***174635-94-0P*** ***174635-95-1P*** ***174635-96-2P*** ***174635-97-3P*** ***174635-98-4P*** ***174636-00-1P*** ***174636-01-2P*** ***174636-03-4P*** ***174636-04-5P*** ***174636-05-6P*** ***174636-06-7P*** ***174636-07-8P*** ***174636-09-0P*** ***174636-10-3P*** ***174636-11-4P*** ***174636-12-5P*** ***174636-13-6P*** ***174636-14-7P*** ***174636-15-8P*** ***174636-16-9P*** ***174636-17-0P*** ***174636-18-1P*** ***174636-19-2P*** ***174636-20-5P*** ***174636-21-6P*** ***174636-22-7P*** ***174636-23-8P*** ***174636-24-9P*** ***174636-25-0P*** ***174636-26-1P*** ***174636-27-2P*** ***174636-28-3P*** ***174636-29-4P*** ***174636-30-7P*** ***174636-31-8P*** ***174636-32-9P*** ***174636-33-0P*** ***174636-34-1P*** ***174636-35-2P*** ***174636-36-3P*** ***174636-37-4P*** ***174636-38-5P*** ***174636-39-6P*** ***174636-40-9P*** ***174636-42-1P*** ***174636-43-2P*** ***174636-44-3P*** ***174636-46-5P*** ***174636-47-6P*** ***174636-49-8P*** ***174636-50-1P*** ***174636-51-2P*** ***174636-52-3P*** ***174636-53-4P*** ***174636-54-5P*** ***174636-55-6P*** ***174636-56-7P*** ***174636-57-8P*** ***174636-58-9P*** ***174636-60-3P*** ***174636-61-4P*** ***174636-62-5P*** ***189815-94-9P*** ***191796-73-3P*** ***191939-91-0P*** ***191939-92-1P***

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinoline-deriv. NK_3 receptor antagonists)

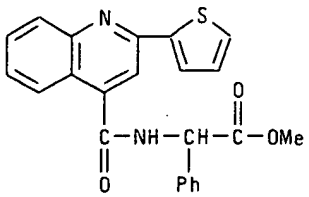
RN 174635-48-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylethyl)- (9CI) (CA INDEX NAME)



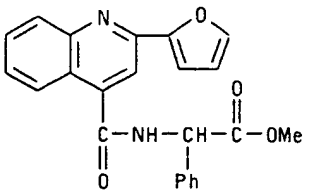
RN 174635-49-5 CA

RN 174635-58-6 CA



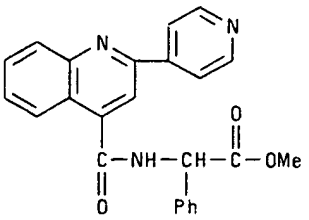
RN 174635-59-7 CA

CN Benzeneacetic acid, α-[[[2-(2-furanyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-60-0 CA

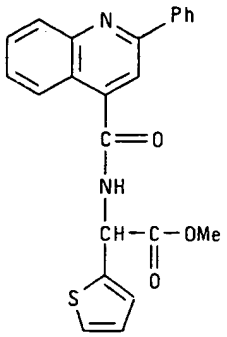
CN Benzeneacetic acid, α-[[[2-(4-pyridinyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-61-1 CA

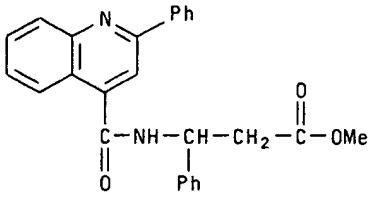
CN 2-Thiopheneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-61-1 CA



RN 174635-62-2 CA

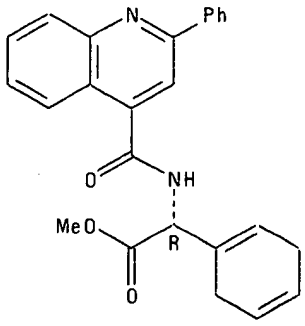
CN Benzenepropanoic acid, β-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-63-3 CA

CN 1,4-Cyclohexadiene-1-acetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

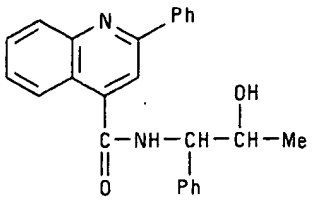
Absolute stereochemistry. Rotation (-).



RN 174635-64-4 CA

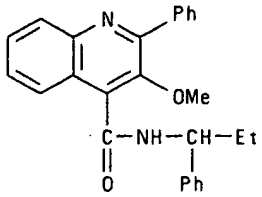
CN 4-Quinolinecarboxamide, *N*-(2-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-64-4 CA



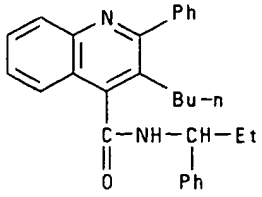
RN 174635-65-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



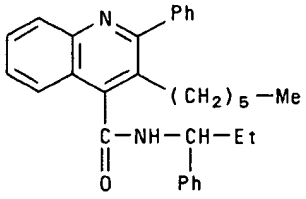
RN 174635-66-6 CA

CN 4-Quinolinecarboxamide, 3-butyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



RN 174635-68-8 CA

CN 4-Quinolinecarboxamide, 3-hexyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

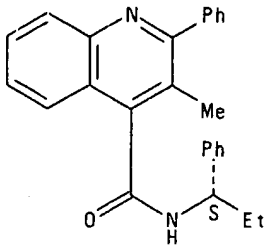


RN 174635-69-9 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

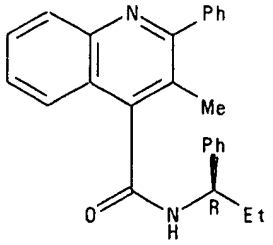
RN 174635-69-9 CA



RN 174635-70-2 CA

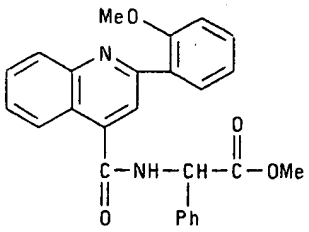
CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 174635-71-3 CA

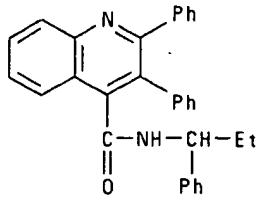
CN Benzeneacetic acid, α-[[[2-(2-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-72-4 CA

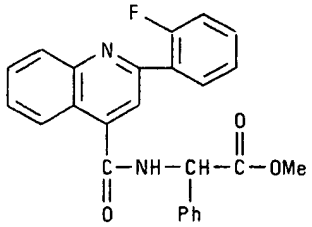
CN 4-Quinolinecarboxamide, 2,3-diphenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-72-4 CA



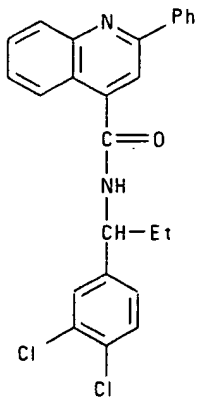
RN 174635-73-5 CA

CN Benzeneacetic acid, α-[[[2-(2-fluorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-74-6 CA

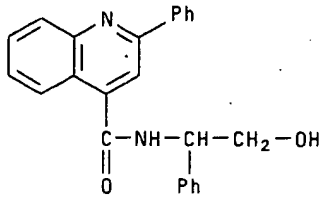
CN 4-Quinolinecarboxamide, *N*-[1-(3,4-dichlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)



RN 174635-75-7 CA

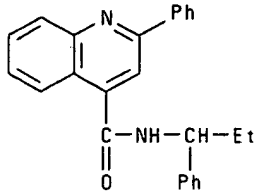
CN 4-Quinolinecarboxamide, *N*-(2-hydroxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-75-7 CA



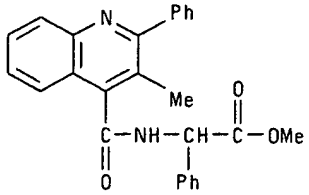
RN 174635-76-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



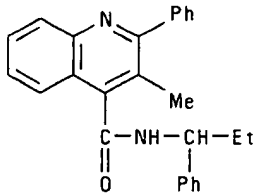
RN 174635-77-9 CA

CN Benzeneacetic acid, α-[[(3-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-78-0 CA

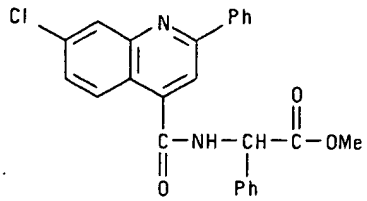
CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



RN 174635-79-1 CA

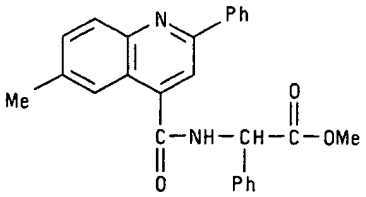
RN 174635-79-1 CA

CN Benzeneacetic acid, α-[[(7-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



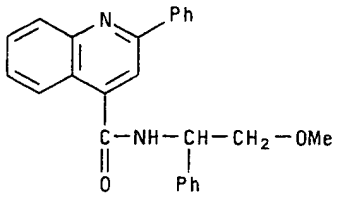
RN 174635-80-4 CA

CN Benzeneacetic acid, α-[[(6-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



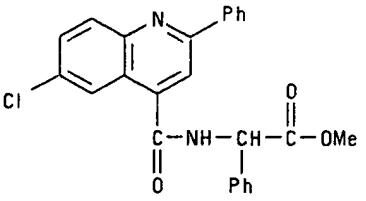
RN 174635-81-5 CA

CN 4-Quinolinecarboxamide, N-(2-methoxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174635-82-6 CA

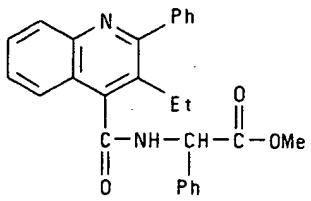
CN Benzeneacetic acid, α-[[(6-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-82-6 CA

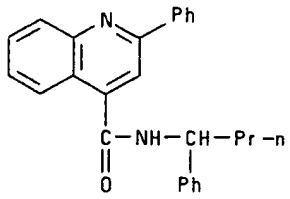
RN 174635-83-7 CA

CN Benzeneacetic acid, α-[[(3-ethyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



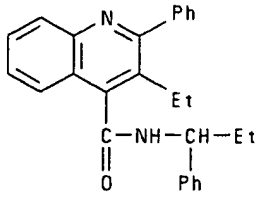
RN 174635-84-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylbutyl)- (9CI) (CA INDEX NAME)



RN 174635-85-9 CA

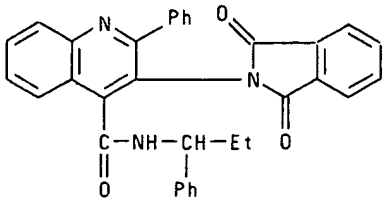
CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



RN 174635-86-0 CA

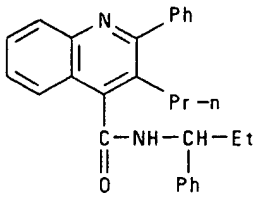
CN 4-Quinolinecarboxamide, 3-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-86-0 CA



RN 174635-87-1 CA

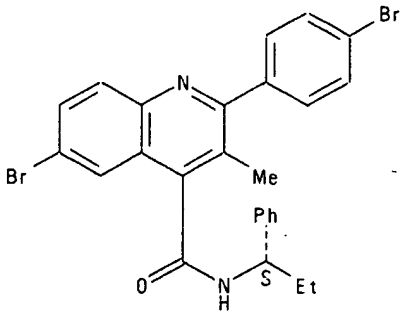
CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-propyl- (9CI) (CA INDEX NAME)



RN 174635-88-2 CA

CN 4-Quinolinecarboxamide, 6-bromo-2-(4-bromophenyl)-3-methyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

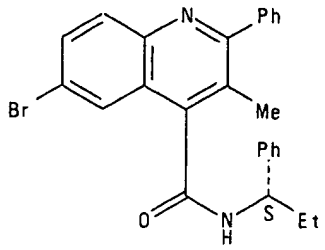


RN 174635-89-3 CA

CN 4-Quinolinecarboxamide, 6-bromo-3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

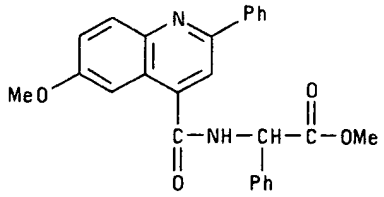
Absolute stereochemistry. Rotation (-).

RN 174635-89-3 CA



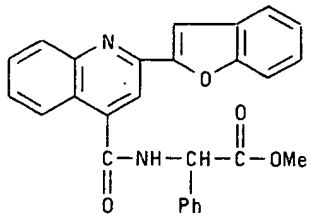
RN 174635-90-6 CA

CN Benzeneacetic acid, α-[[(6-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



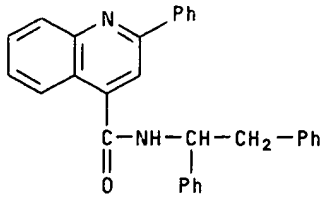
RN 174635-91-7 CA

CN Benzeneacetic acid, α-[[[2-(2-benzofuranyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-92-8 CA

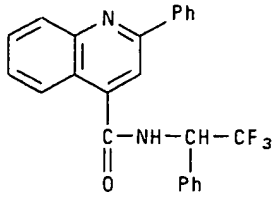
CN 4-Quinolinecarboxamide, *N*-(1,2-diphenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174635-93-9 CA

RN 174635-93-9 CA

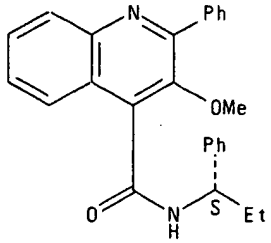
CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(2,2,2-trifluoro-1-phenylethyl)- (9CI) (CA INDEX NAME)



RN 174635-94-0 CA

CN 4-Quinolinecarboxamide, 3-methoxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

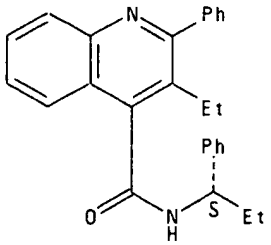
Absolute stereochemistry. Rotation (-).



RN 174635-95-1 CA

CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

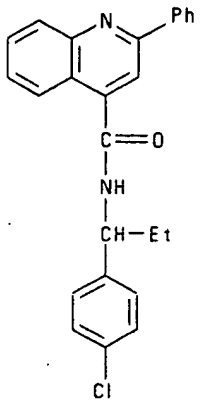
Absolute stereochemistry. Rotation (-).



RN 174635-96-2 CA

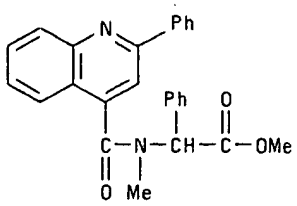
CN 4-Quinolinecarboxamide, *N*-[1-(4-chlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-96-2 CA



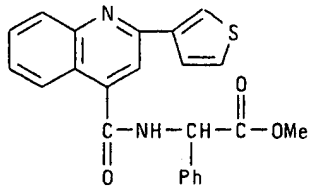
RN 174635-97-3 CA

CN Benzeneacetic acid, α-[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-98-4 CA

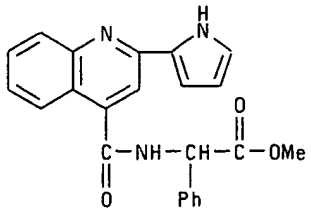
CN Benzeneacetic acid, α-[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-00-1 CA

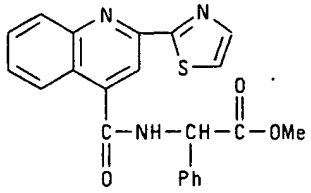
CN Benzeneacetic acid, α-[[[2-(1*H*-pyrrol-2-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-00-1 CA



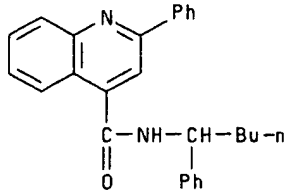
RN 174636-01-2 CA

CN Benzeneacetic acid, α-[[[2-(2-thiazolyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



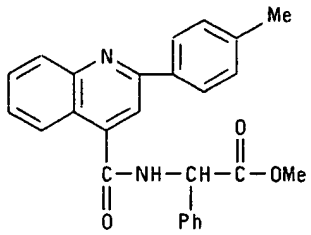
RN 174636-03-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpentyl)- (9CI) (CA INDEX NAME)



RN 174636-04-5 CA

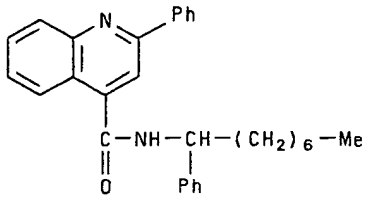
CN Benzeneacetic acid, α-[[[2-(4-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-05-6 CA

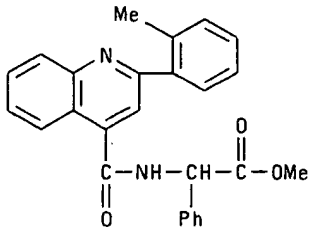
RN 174636-05-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenyloctyl)- (9CI) (CA INDEX NAME)



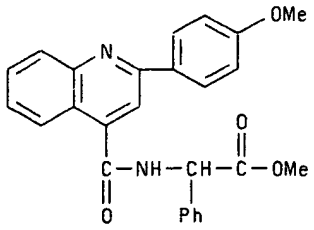
RN 174636-06-7 CA

CN Benzeneacetic acid, α-[[[2-(2-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-07-8 CA

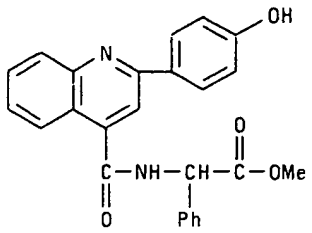
CN Benzeneacetic acid, α-[[[2-(4-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-09-0 CA

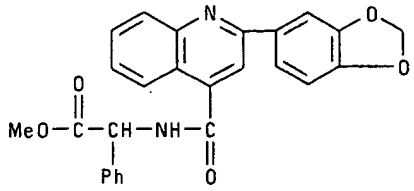
CN Benzeneacetic acid, α-[[[2-(4-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-09-0 CA



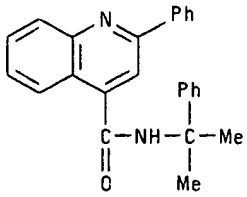
RN 174636-10-3 CA

CN Benzeneacetic acid, α-[[[2-(1,3-benzodioxol-5-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-11-4 CA

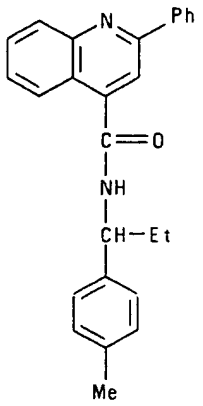
CN 4-Quinolinecarboxamide, *N*-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-12-5 CA

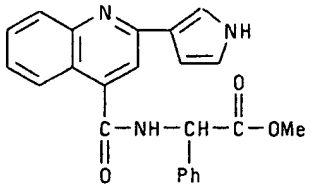
CN 4-Quinolinecarboxamide, *N*-[1-(4-methylphenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-12-5 CA



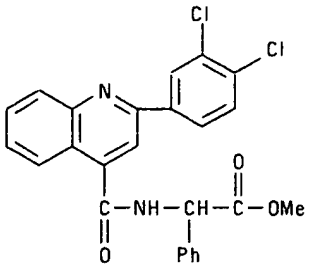
RN 174636-13-6 CA

CN Benzeneacetic acid, α-[[[2-(1*H*-pyrrol-3-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-14-7 CA

CN Benzeneacetic acid, α-[[[2-(3,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

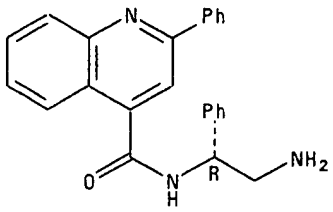


RN 174636-15-8 CA

CN 4-Quinolinecarboxamide, *N*-(2-amino-1-phenylethyl)-2-phenyl-, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

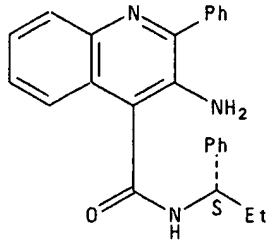
RN 174636-15-8 CA



RN 174636-16-9 CA

CN 4-Quinolinecarboxamide, 3-amino-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

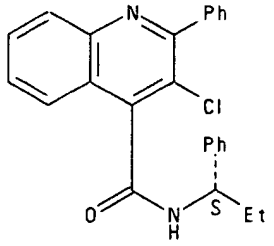
Absolute stereochemistry. Rotation (-).



RN 174636-17-0 CA

CN 4-Quinolinecarboxamide, 3-chloro-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

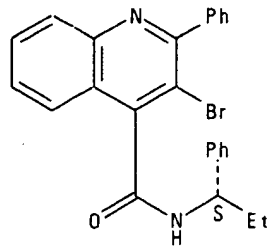


RN 174636-18-1 CA

CN 4-Quinolinecarboxamide, 3-bromo-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

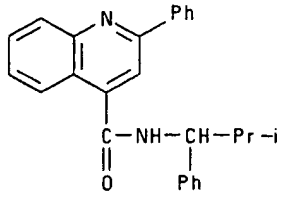
Absolute stereochemistry. Rotation (-).

RN 174636-18-1 CA



RN 174636-19-2 CA

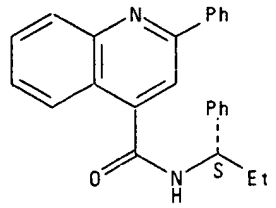
CN 4-Quinolinecarboxamide, *N*-(2-methyl-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-20-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

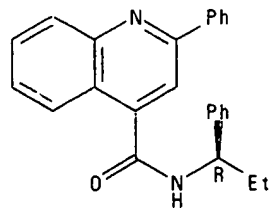
Absolute stereochemistry. Rotation (-).



RN 174636-21-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-, (*R*)- (9CI) (CA INDEX NAME)

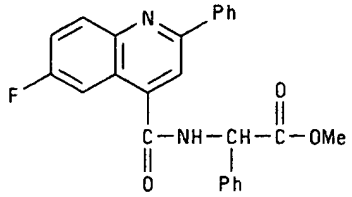
Absolute stereochemistry. Rotation (+).



RN 174636-22-7 CA

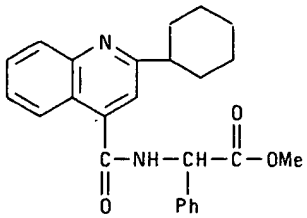
RN 174636-22-7 CA

CN Benzeneacetic acid, α-[[(6-fluoro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



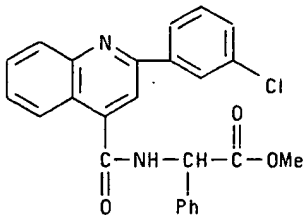
RN 174636-23-8 CA

CN Benzeneacetic acid, α-[[(2-cyclohexyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-24-9 CA

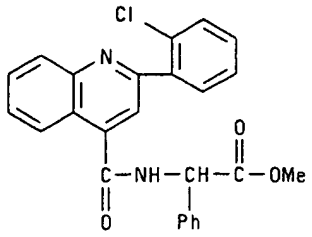
CN Benzeneacetic acid, α-[[[2-(3-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-25-0 CA

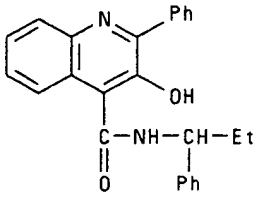
CN Benzeneacetic acid, α-[[[2-(2-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-25-0 CA



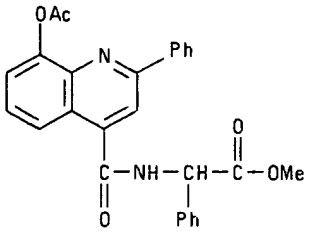
RN 174636-26-1 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



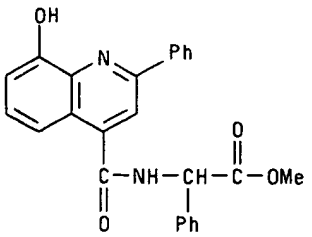
RN 174636-27-2 CA

CN Benzeneacetic acid, α-[[[8-(acetyloxy)-2-phenyl-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-28-3 CA

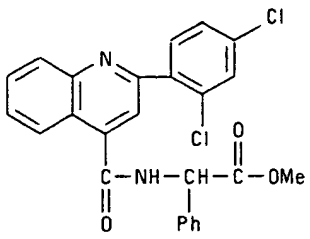
CN Benzeneacetic acid, α-[[(8-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-28-3 CA

RN 174636-29-4 CA

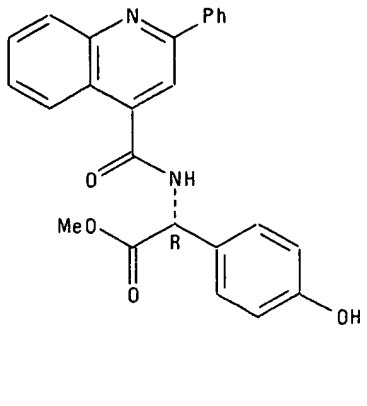
CN Benzeneacetic acid, α-[[[2-(2,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-30-7 CA

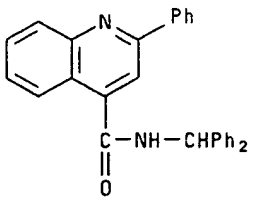
CN Benzeneacetic acid, 4-hydroxy-α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, monohydrochloride, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 174636-31-8 CA

CN 4-Quinolinecarboxamide, *N*-(diphenylmethyl)-2-phenyl- (9CI) (CA INDEX NAME)

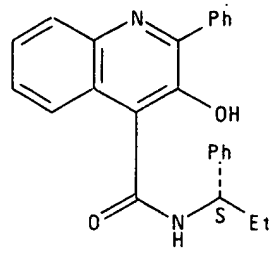


RN 174636-32-9 CA

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

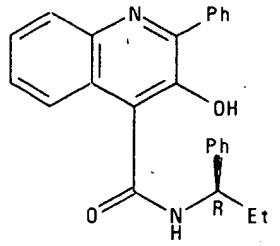
Absolute stereochemistry. Rotation (-).



RN 174636-33-0 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*R*)- (9CI) (CA INDEX NAME)

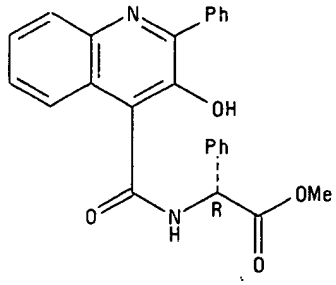
Absolute stereochemistry. Rotation (+).



RN 174636-34-1 CA

CN Benzeneacetic acid, α-[[(3-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

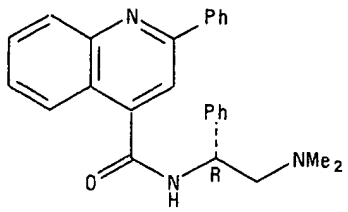


RN 174636-35-2 CA

CN 4-Quinolinecarboxamide, *N*-[2-(dimethylamino)-1-phenylethyl]-2-phenyl-, (*R*)- (9CI) (CA INDEX NAME)

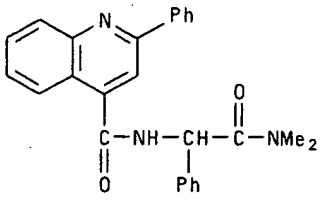
RN 174636-35-2 CA

Absolute stereochemistry. Rotation (-).



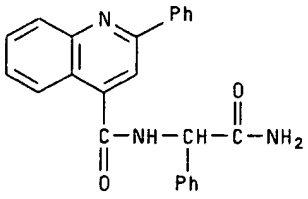
RN 174636-36-3 CA

CN 4-Quinolinecarboxamide, *N*-[2-(dimethylamino)-2-oxo-1-phenylethyl]-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-37-4 CA

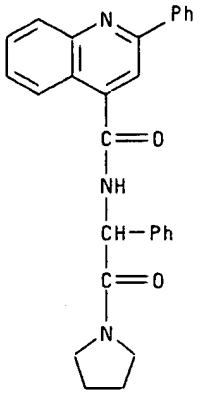
CN 4-Quinolinecarboxamide, *N*-(2-amino-2-oxo-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-38-5 CA

CN 4-Quinolinecarboxamide, *N*-[2-oxo-1-phenyl-2-(1-pyrrolidinyl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

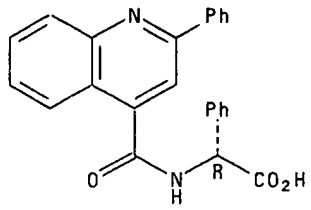
RN 174636-38-5 CA



RN 174636-39-6 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride, (*R*)- (9CI) (CA INDEX NAME)

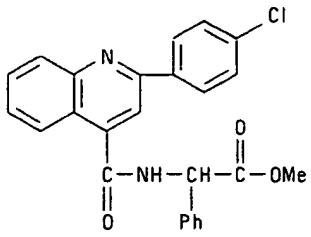
Absolute stereochemistry. Rotation (-).



• HCl

RN 174636-40-9 CA

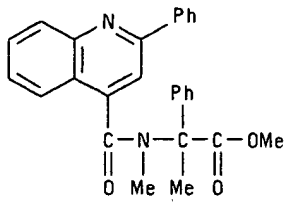
CN Benzeneacetic acid, α-[[[2-(4-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-42-1 CA

RN 174636-42-1 CA

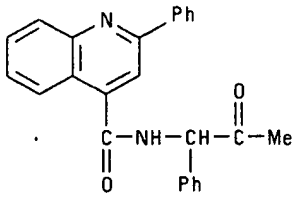
CN Benzeneacetic acid, α-methyl-α-[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



• HCl

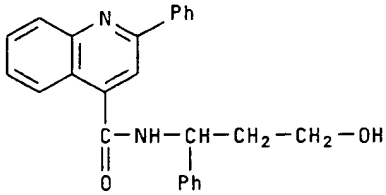
RN 174636-43-2 CA

CN 4-Quinolinecarboxamide, *N*-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-44-3 CA

CN 4-Quinolinecarboxamide, *N*-(3-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

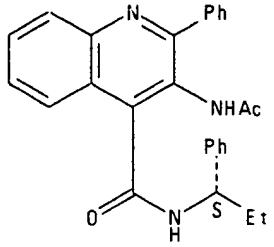


RN 174636-46-5 CA

CN 4-Quinolinecarboxamide, 3-(acetylamino)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

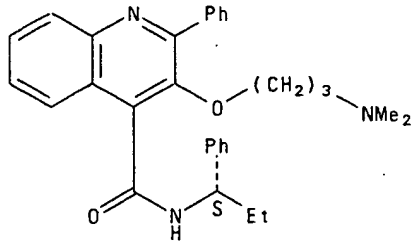
RN 174636-46-5 CA



RN 174636-47-6 CA

CN 4-Quinolinecarboxamide, 3-[3-(dimethylamino)propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

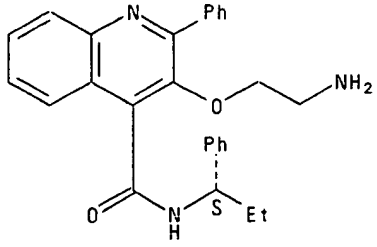


• HCl

RN 174636-49-8 CA

CN 4-Quinolinecarboxamide, 3-(2-aminoethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



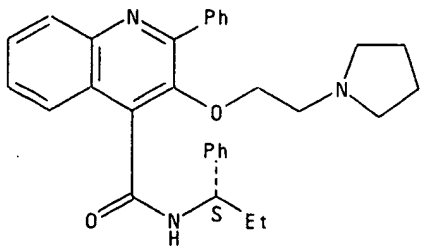
• HCl

RN 174636-50-1 CA

RN 174636-50-1 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-(1-pyrrolidinyl)ethoxy]-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

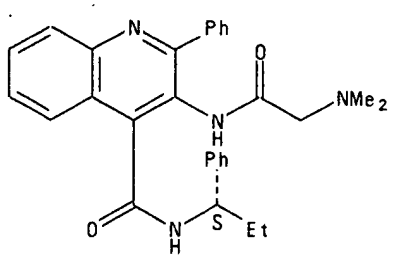


• HCl

RN 174636-51-2 CA

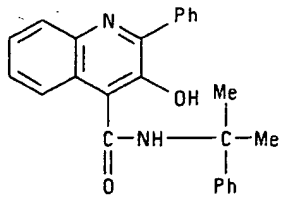
CN 4-Quinolinecarboxamide, 3-[[(dimethylamino)acetyl]amino]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 174636-52-3 CA

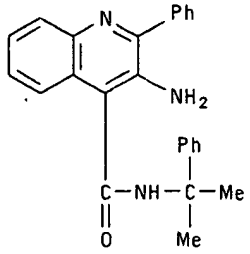
CN 4-Quinolinecarboxamide, 3-hydroxy-*N*-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-53-4 CA

CN 4-Quinolinecarboxamide, 3-amino-*N*-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

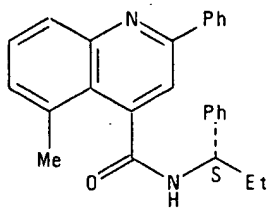
RN 174636-53-4 CA



RN 174636-54-5 CA

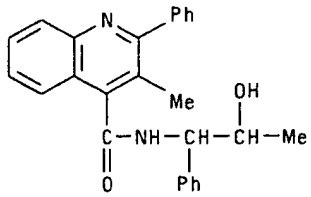
CN 4-Quinolinecarboxamide, 5-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



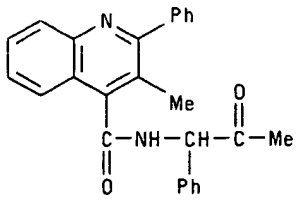
RN 174636-55-6 CA

CN 4-Quinolinecarboxamide, *N*-(2-hydroxy-1-phenylpropyl)-3-methyl-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-56-7 CA

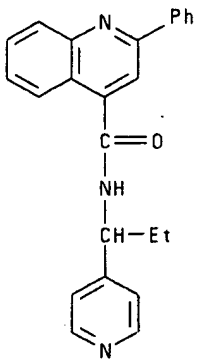
CN 4-Quinolinecarboxamide, 3-methyl-*N*-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-57-8 CA

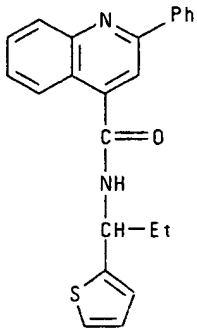
RN 174636-57-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-[1-(4-pyridinyl)propyl]- (9CI) (CA INDEX NAME)



RN 174636-58-9 CA

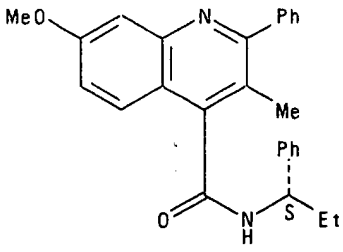
CN 4-Quinolinecarboxamide, 2-phenyl-*N*-[1-(2-thienyl)propyl]- (9CI) (CA INDEX NAME)



RN 174636-60-3 CA

CN 4-Quinolinecarboxamide, 7-methoxy-3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

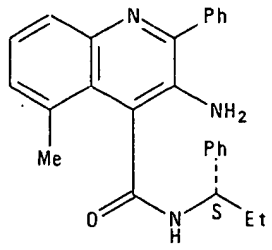


RN 174636-61-4 CA

RN 174636-61-4 CA

CN 4-Quinolinecarboxamide, 3-amino-5-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

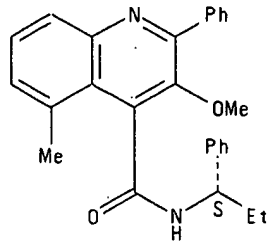
Absolute stereochemistry.



RN 174636-62-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-5-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

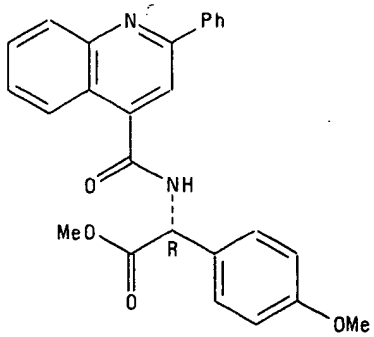
Absolute stereochemistry.



RN 189815-94-9 CA

CN Benzeneacetic acid, 4-methoxy-α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

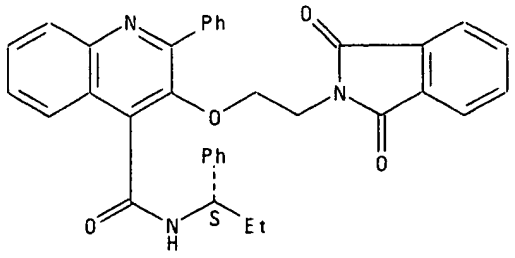


RN 189815-94-9 CA

RN 191796-73-3 CA

CN 4-Quinolinecarboxamide, 3-[2-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

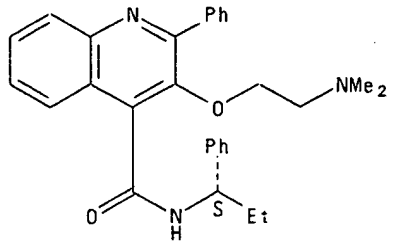
Absolute stereochemistry. Rotation (-).



RN 191939-91-0 CA

CN 4-Quinolinecarboxamide, 3-[2-(dimethylamino)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

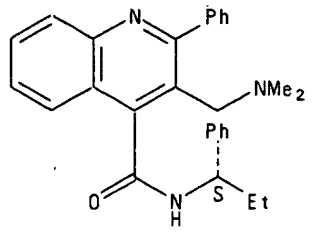


RN 191939-92-1 CA

CN 4-Quinolinecarboxamide, 3-[(dimethylamino)methyl]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 191939-92-1 CA



• HCl

****

L6 ANSWER 4 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 4

AN 127:95204 CA

TI Preparation of quinoline-4-carboxamides and their use as neurokinin-3 and neurokinin-2 receptor antagonists

IN Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farina, Carlo

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farina, Carlo

SO PCT Int. Appl., 79 pp.
CODEN: PIXXD2

PI WO 9719926 A1 970605

DS TT, W UA, W UG, W US, W UZ, W VN, W AM, W AZ, W BY, W KG, W KZ, W MD, W RU, W TJ, W TM, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 96-EP5207 961122

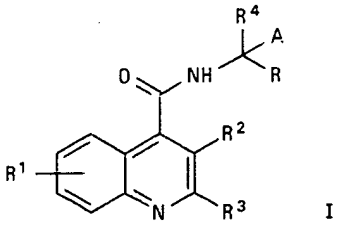
PRAI IT 95-MI2462 951124
IT 96-MI1688 960802

DT Patent

LA English

OS MARPAT 127:95204

GI



I

AB The title compds. [I; A = (un)substituted aryl, C_{5-7} cycloalkdienyl, (un)substituted single or fused ring arom. heterocyclyl; R = (un)substituted C_{1-6} alkyl, C_{3-7} cycloalkyl, C_{3-7} cycloalkylalkyl, (un)substituted Ph, an optionally substituted five-membered heteroarom. ring, etc.; R^1 = hydrogen or up to four substituents selected from C_{1-6} alkyl, C_{1-6} alkenyl, aryl, C_{1-6} alkoxy, hydroxy, halogen, nitro, cyano, carboxy, carboxamido, sulfonamido, C_{1-6} alkoxycarbonyl, trifluoromethyl, alkoxy, phthalimido, (un)substituted amino, etc.; R^2 = hydrogen, C_{1-6} alkyl, hydroxy, halogen, cyano, (un)substituted amino, etc.; R^3 = C_{1-6} alkyl, C_{3-7} cycloalkyl, C_{4-7} cycloalkylalkyl, (un)substituted aryl, (un)substituted single or fused ring arom. heterocyclyl; R^4 = hydrogen, C_{1-6} alkyl], useful as neurokinin 3 and neurokinin 2 receptor antagonists, are prepd.

L6 ANSWER 4 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 4

Thus, (S)-N-(α-ethylbenzyl)-3-(2-aminoethoxy)-2-phenylquinoline-4-carboxamide was reacted with α,α'-dibromo-o-xylene and salified with HCl, producing (S)-N-(α-ethylbenzyl)-3-[2-(2-isoindolinyl)ethoxy]-2-phenylquinoline-4-carboxamide dihydrochloride (m.p. 95°; decompn.) which demonstrated a binding affinity in human neurokinin-3 receptors (expressed in CHO cell lines) against [^{125}I]-[Me-Phe^{7}]-neurokinin B of 1.2 nM.

IT ***191796-25-5P*** ***191796-26-6P*** ***191796-27-7P*** ***191796-28-8P*** ***191796-29-9P*** ***191796-30-2P*** ***191796-31-3P*** ***191796-32-4P*** ***191796-33-5P*** ***191796-34-6P*** ***191796-35-7P*** ***191796-36-8P*** ***191796-37-9P*** ***191796-38-0P*** ***191796-39-1P*** ***191796-40-4P*** ***191796-41-5P*** ***191796-42-6P*** ***191796-43-7P*** ***191796-44-8P*** ***191796-45-9P*** ***191796-46-0P*** ***191796-47-1P*** ***191796-48-2P*** ***191796-49-3P*** ***191796-50-6P*** ***191796-51-7P*** ***191796-52-8P*** ***191796-53-9P*** ***191796-54-0P*** ***191796-55-1P*** ***191796-56-2P*** ***191796-57-3P*** ***191796-58-4P*** ***191796-59-5P*** ***191796-60-8P*** ***191796-61-9P*** ***191796-62-0P*** ***191796-63-1P*** ***191796-64-2P*** ***191796-65-3P*** ***191796-66-4P*** ***191796-67-5P*** ***191796-68-6P*** ***191796-69-7P*** ***191796-70-0P***

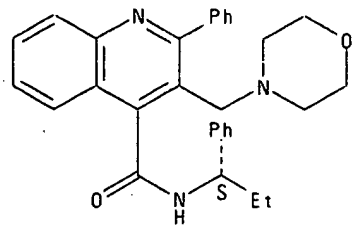
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinoline-4-carboxamides and their use as neurokinin-3 and neurokinin-2 receptor antagonists)

RN 191796-25-5 CA

CN 4-Quinolinecarboxamide, 3-(4-morpholinylmethyl)-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



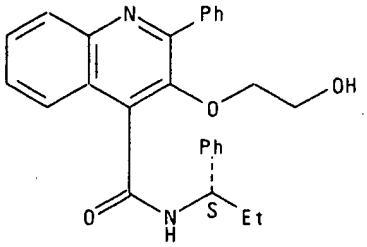
• HCl

RN 191796-26-6 CA

RN 191796-26-6 CA

CN 4-Quinolinecarboxamide, 3-(2-hydroxyethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

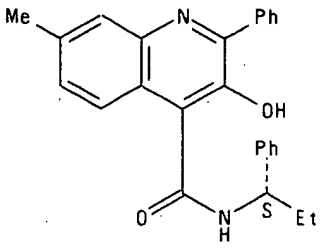
Absolute stereochemistry. Rotation (-).



RN 191796-27-7 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-7-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

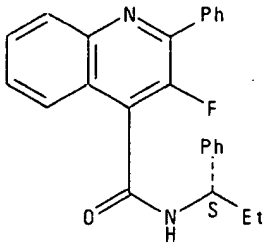
Absolute stereochemistry.



RN 191796-28-8 CA

CN 4-Quinolinecarboxamide, 3-fluoro-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

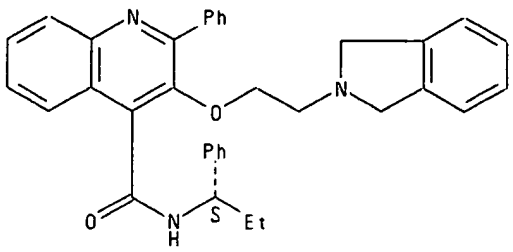


RN 191796-29-9 CA

CN 4-Quinolinecarboxamide, 3-[2-(1,3-dihydro-2*H*-isoindol-2-yl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, dihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

RN 191796-29-9 CA

Absolute stereochemistry.

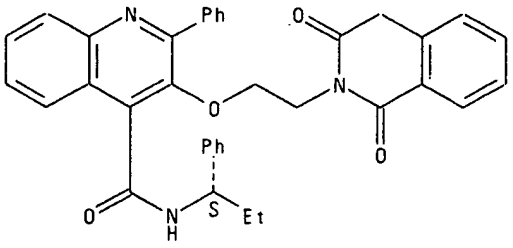


• 2 HCl

RN 191796-30-2 CA

CN 4-Quinolinecarboxamide, 3-[2-(3,4-dihydro-1,3-dioxo-2(1*H*)-isoquinolinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

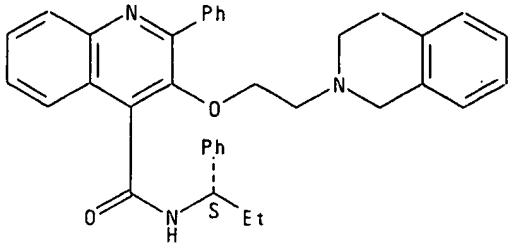


RN 191796-31-3 CA

CN 4-Quinolinecarboxamide, 3-[2-(3,4-dihydro-2(1*H*)-isoquinolinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

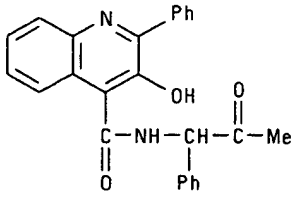
RN 191796-31-3 CA



• HCl

RN 191796-32-4 CA

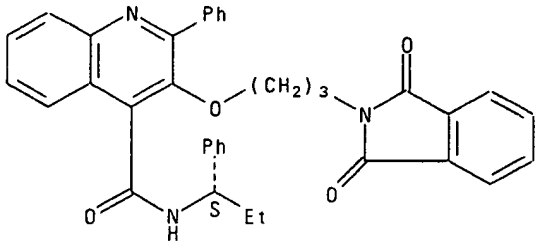
CN 4-Quinolinecarboxamide, 3-hydroxy-*N*-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 191796-33-5 CA

CN 4-Quinolinecarboxamide, 3-[3-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

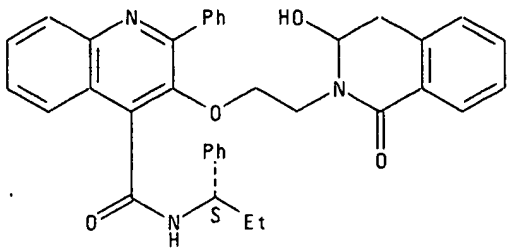


RN 191796-34-6 CA

CN 4-Quinolinecarboxamide, 3-[2-(3,4-dihydro-3-hydroxy-1-oxo-2(1*H*)-isoquinolinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [2(*S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

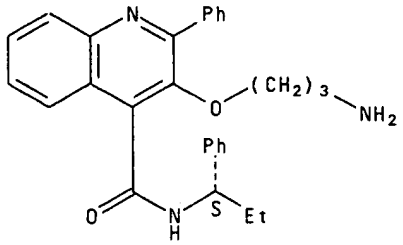
RN 191796-34-6 CA



RN 191796-35-7 CA

CN 4-Quinolinecarboxamide, 3-(3-aminopropoxy)-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

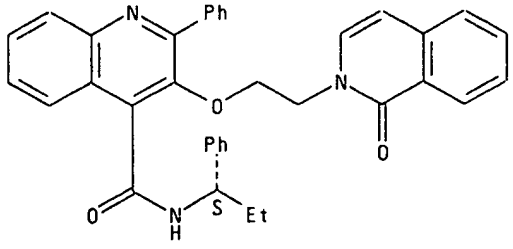


• HCl

RN 191796-36-8 CA

CN 4-Quinolinecarboxamide, 3-[2-(1-oxo-2(1*H*)-isoquinolinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

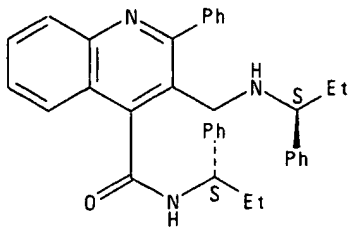


RN 191796-37-9 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[[(1-phenylpropyl)amino]methyl]-, monohydrochloride, [*S*-(*R**,*R**)]- (9CI) (CA INDEX NAME)

RN 191796-37-9 CA

Absolute stereochemistry. Rotation (-).

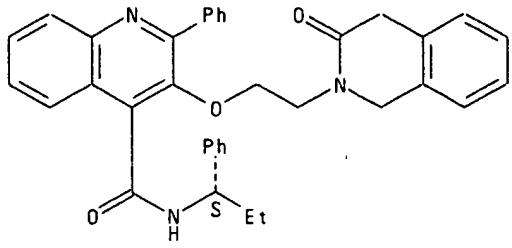


• HCl

RN 191796-38-0 CA

CN 4-Quinolinecarboxamide, 3-[2-(3,4-dihydro-3-oxo-2(1*H*)-isoquinolinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

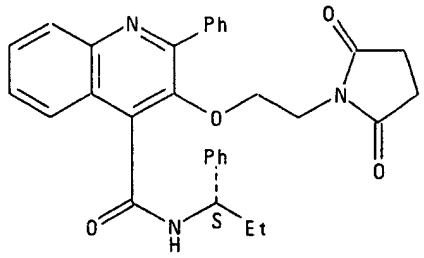
Absolute stereochemistry. Rotation (-).



RN 191796-39-1 CA

CN 4-Quinolinecarboxamide, 3-[2-(2,5-dioxo-1-pyrrolidinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

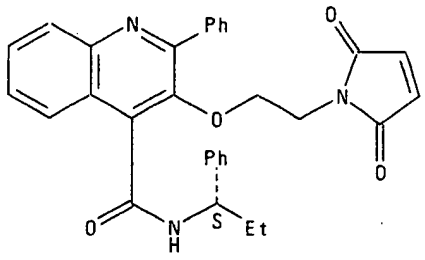


RN 191796-40-4 CA

RN 191796-40-4 CA

CN 4-Quinolinecarboxamide, 3-[2-(2,5-dihydro-2,5-dioxo-1*H*-pyrrol-1-yl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

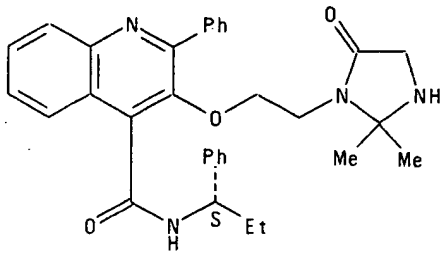
Absolute stereochemistry. Rotation (-).



RN 191796-41-5 CA

CN 4-Quinolinecarboxamide, 3-[2-(2,2-dimethyl-5-oxo-1-imidazolidinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

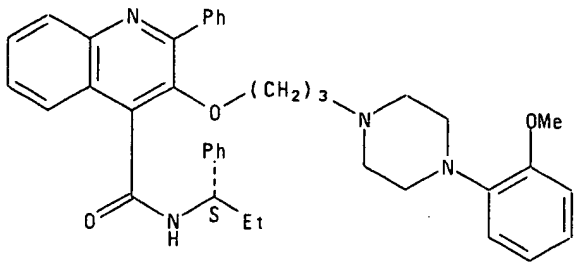


RN 191796-42-6 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, dihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-42-6 CA

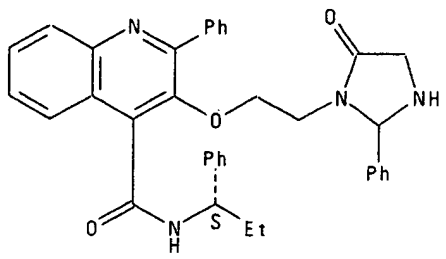


• 2 HCl

RN 191796-43-7 CA

CN 4-Quinolinecarboxamide, 3-[2-(5-oxo-2-phenyl-1-imidazolidinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [1(*S*)]- (9CI) (CA INDEX NAME)

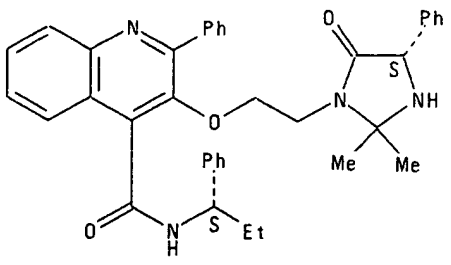
Absolute stereochemistry.



RN 191796-44-8 CA

CN 4-Quinolinecarboxamide, 3-[2-(2,2-dimethyl-5-oxo-4-phenyl-1-imidazolidinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [*S*-(*R**,*R**)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

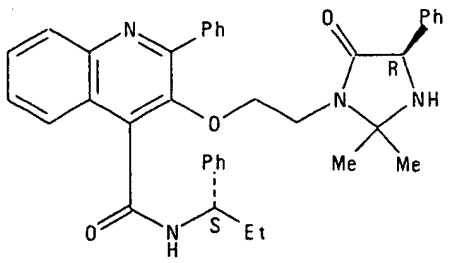


RN 191796-45-9 CA

RN 191796-45-9 CA

CN 4-Quinolinecarboxamide, 3-[2-(2,2-dimethyl-5-oxo-4-phenyl-1-imidazolidinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [*S*-(*R**,*S**)]- (9CI) (CA INDEX NAME)

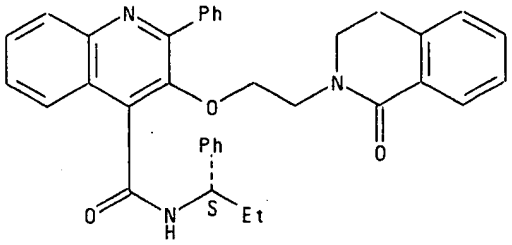
Absolute stereochemistry. Rotation (-).



RN 191796-46-0 CA

CN 4-Quinolinecarboxamide, 3-[2-(3,4-dihydro-1-oxo-2(1*H*)-isoquinolinyl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

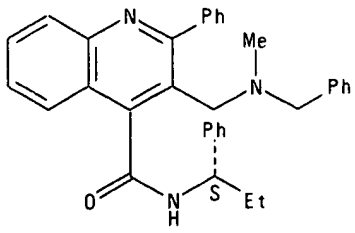
Absolute stereochemistry. Rotation (-).



RN 191796-47-1 CA

CN 4-Quinolinecarboxamide, 3-[[methyl(phenylmethyl)amino]methyl]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

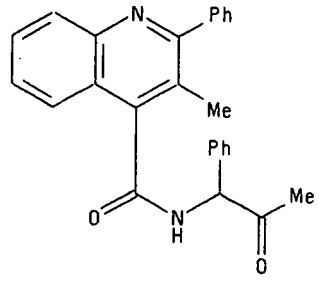


RN 191796-48-2 CA

RN 191796-48-2 CA

CN 4-Quinolinecarboxamide, 3-methyl-*N*-(2-oxo-1-phenylpropyl)-2-phenyl-, (-)- (9CI) (CA INDEX NAME)

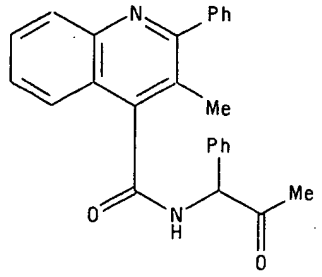
Rotation (-).



RN 191796-49-3 CA

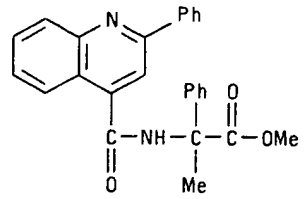
CN 4-Quinolinecarboxamide, 3-methyl-*N*-(2-oxo-1-phenylpropyl)-2-phenyl-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



RN 191796-50-6 CA

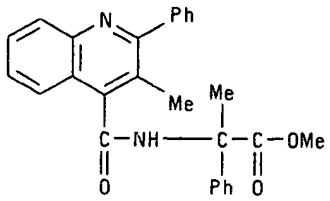
CN Benzeneacetic acid, α-methyl-α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 191796-51-7 CA

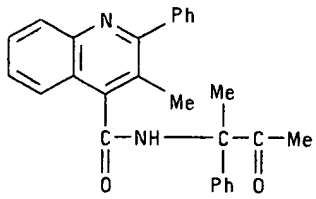
CN Benzeneacetic acid, α-methyl-α-[[(3-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 191796-51-7 CA



RN 191796-52-8 CA

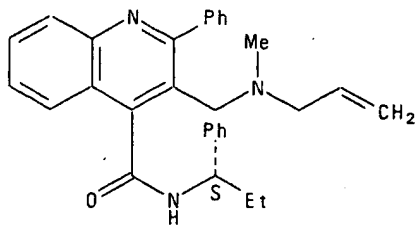
CN 4-Quinolinecarboxamide, 3-methyl-*N*-(1-methyl-2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 191796-53-9 CA

CN 4-Quinolinecarboxamide, 3-[(methyl-2-propenylamino)methyl]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

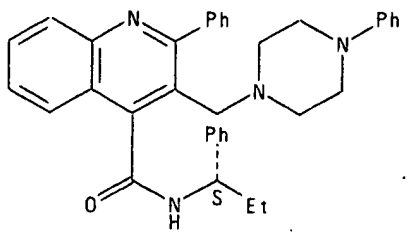


RN 191796-54-0 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[(4-phenyl-1-piperazinyl)methyl]-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

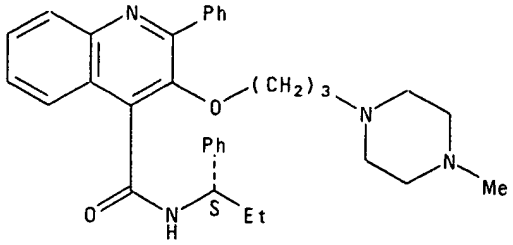
RN 191796-54-0 CA



RN 191796-55-1 CA

CN 4-Quinolinecarboxamide, 3-[3-(4-methyl-1-piperazinyl)propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, trihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

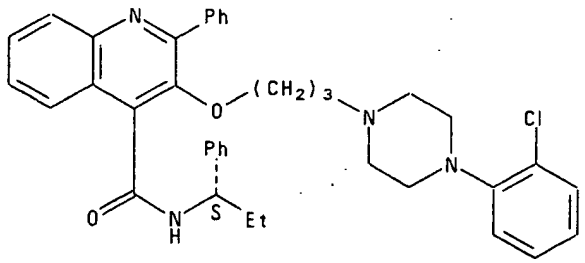


• 3 HCl

RN 191796-56-2 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(2-chlorophenyl)-1-piperazinyl]propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, dihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



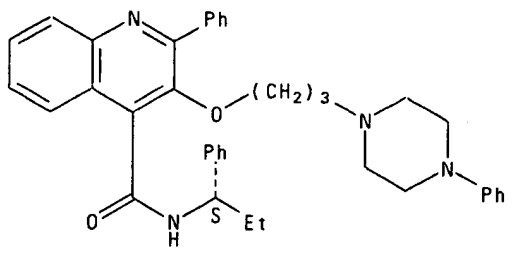
• 2 HCl

RN 191796-57-3 CA

RN 191796-57-3 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[3-(4-phenyl-1-piperazinyl)propoxy]-*N*-(1-phenylpropyl)-, hydrochloride (2:5), (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

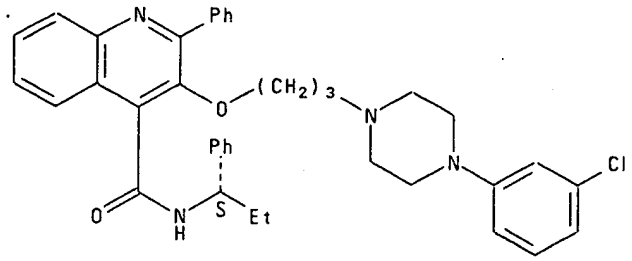


• 5/2 HCl

RN 191796-58-4 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(3-chlorophenyl)-1-piperazinyl]propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, dihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



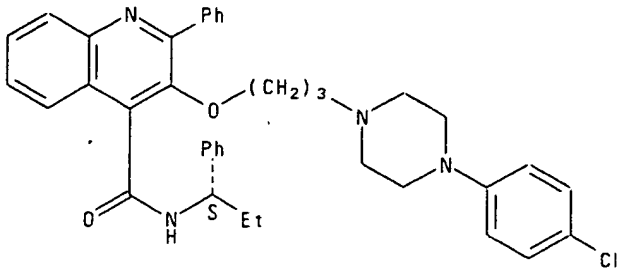
• 2 HCl

RN 191796-59-5 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(4-chlorophenyl)-1-piperazinyl]propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, dihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-59-5 CA

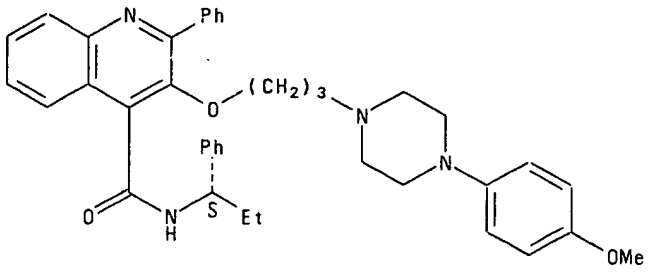


• 2 HCl

RN 191796-60-8 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(4-methoxyphenyl)-1-piperazinyl]propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, dihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



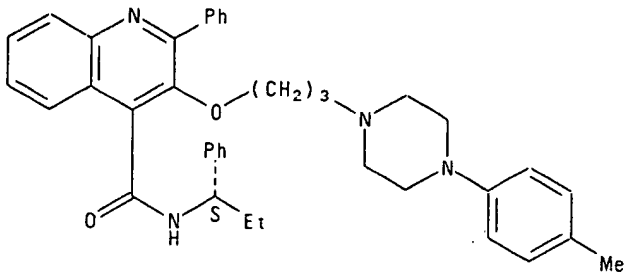
• 2 HCl

RN 191796-61-9 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(4-methylphenyl)-1-piperazinyl]propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, hydrochloride (2:5), (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-61-9 CA

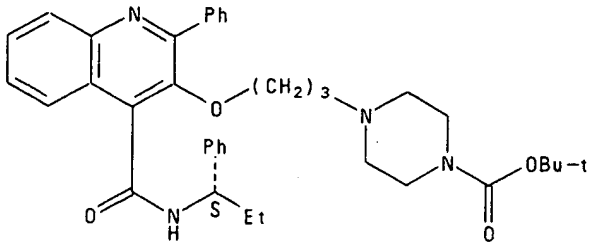


• 5/2 HCl

RN 191796-62-0 CA

CN 1-Piperazinecarboxylic acid, 4-[3-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]propyl]-, 1,1-dimethylethyl ester, (*S*)- (9CI) (CA INDEX NAME)

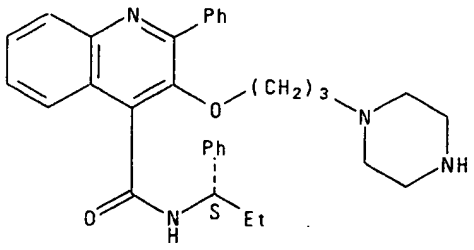
Absolute stereochemistry. Rotation (-).



RN 191796-63-1 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[3-(1-piperazinyl)propoxy]-, trihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



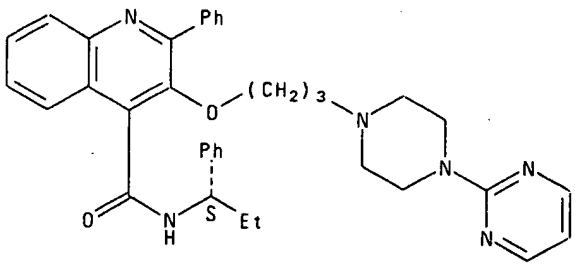
• 3 HCl

RN 191796-63-1 CA

RN 191796-64-2 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[3-[4-(2-pyrimidinyl)-1-piperazinyl]propoxy]-, hydrochloride (2:5), (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

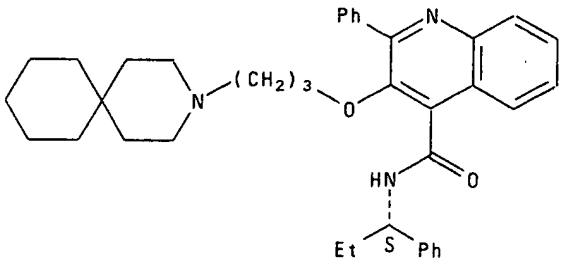


• 5/2 HCl

RN 191796-65-3 CA

CN 4-Quinolinecarboxamide, 3-[3-(3-azaspiro[5.5]undec-3-yl)propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



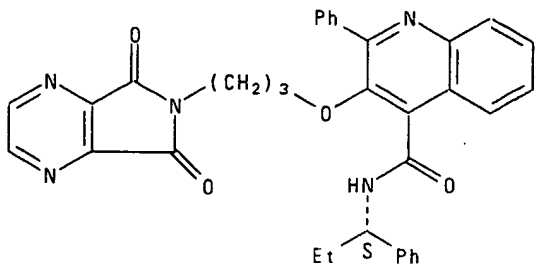
• HCl

RN 191796-66-4 CA

CN 4-Quinolinecarboxamide, 3-[3-(5,7-dihydro-5,7-dioxo-6*H*-pyrrolo[3,4-*b*]pyrazin-6-yl)propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

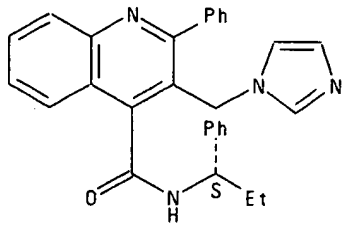
RN 191796-66-4 CA



RN 191796-67-5 CA

CN 4-Quinolinecarboxamide, 3-(1*H*-imidazol-1-ylmethyl)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

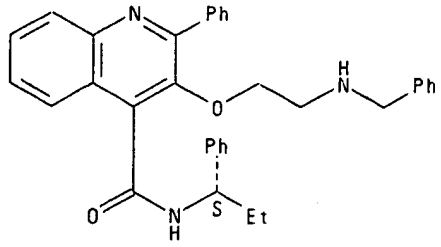
Absolute stereochemistry. Rotation (-).



RN 191796-68-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(phenylmethyl)amino]ethoxy]-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



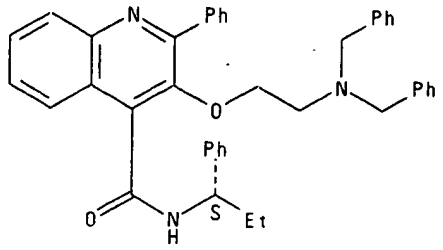
• HCl

RN 191796-69-7 CA

CN 4-Quinolinecarboxamide, 3-[2-[bis(phenylmethyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

RN 191796-69-7 CA

Absolute stereochemistry. Rotation (-).

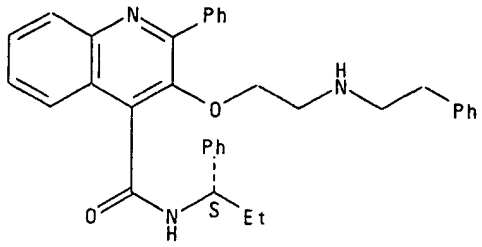


• HCl

RN 191796-70-0 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(2-phenylethyl)amino]ethoxy]-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



• HCl

IT ***174636-32-9P*** ***191796-72-2P*** ***191796-73-3P*** ***191796-74-4P*** ***191796-75-5P*** ***191796-76-6P*** ***191796-77-7P*** ***191796-78-8P*** ***191796-79-9P*** ***191796-80-2P*** ***191796-81-3P*** ***191796-82-4P*** ***191796-88-0P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

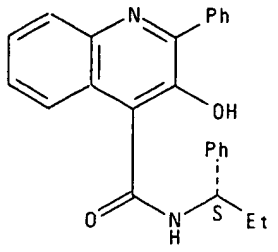
(prepn. of quinoline-4-carboxamides and their use as neurokinin-3 and neurokinin-2 receptor antagonists)

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

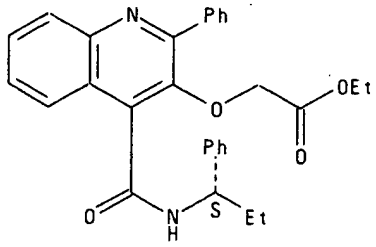
RN 174636-32-9 CA



RN 191796-72-2 CA

CN Acetic acid, [[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, ethyl ester, (*S*)- (9CI) (CA INDEX NAME)

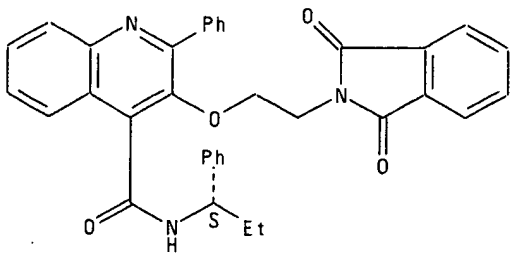
Absolute stereochemistry. Rotation (-).



RN 191796-73-3 CA

CN 4-Quinolinecarboxamide, 3-[2-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

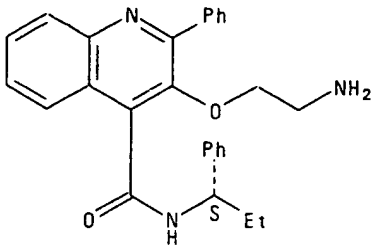


RN 191796-74-4 CA

CN 4-Quinolinecarboxamide, 3-(2-aminoethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

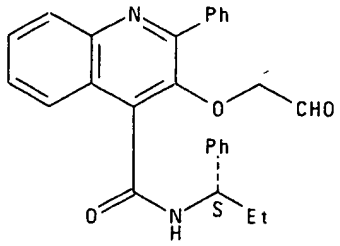
RN 191796-74-4 CA



RN 191796-75-5 CA

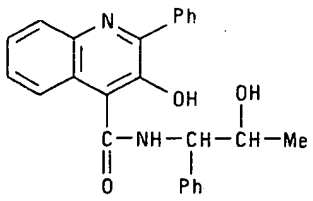
CN 4-Quinolinecarboxamide, 3-(2-oxoethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 191796-76-6 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-*N*-(2-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

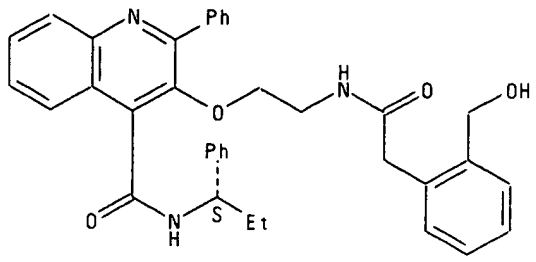


RN 191796-77-7 CA

CN 4-Quinolinecarboxamide, 3-[2-[[[2-(hydroxymethyl)phenyl]acetyl]amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

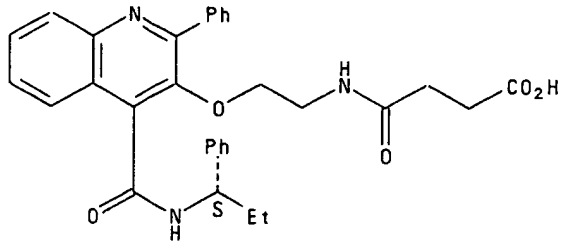
RN 191796-77-7 CA



RN 191796-78-8 CA

CN Butanoic acid, 4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

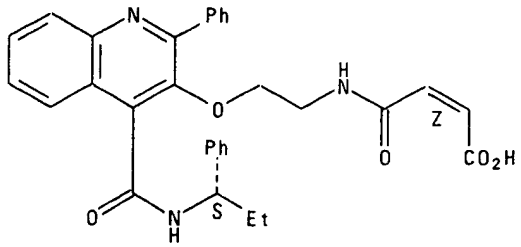


RN 191796-79-9 CA

CN 2-Butenoic acid, 4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, [*S*-(*Z*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

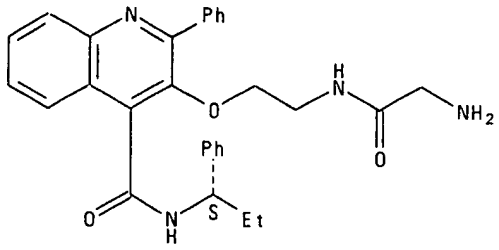


RN 191796-80-2 CA

RN 191796-80-2 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminoacetyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

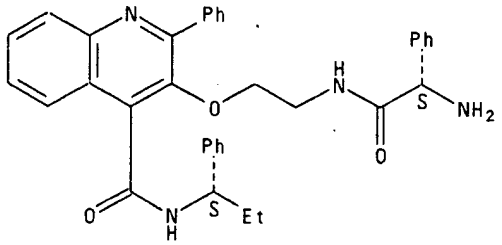
Absolute stereochemistry. Rotation (-).



RN 191796-81-3 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [*S*-(*R**,*R**)]- (9CI) (CA INDEX NAME)

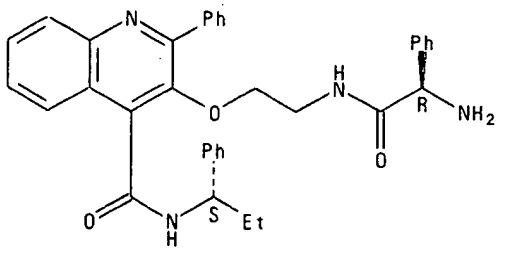
Absolute stereochemistry. Rotation (-).



RN 191796-82-4 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, [*S*-(*R**,*S**)]- (9CI) (CA INDEX NAME)

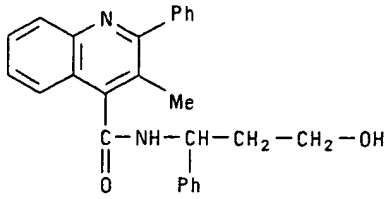
Absolute stereochemistry. Rotation (-).



RN 191796-88-0 CA

RN 191796-88-0 CA

CN 4-Quinolinecarboxamide, *N*-(3-hydroxy-1-phenylpropyl)-3-methyl-2-phenyl- (9CI) (CA INDEX NAME)



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L6 ANSWER 5 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 5

AN 126:338400 CA

TI Discovery of a Novel Class of Selective Non-Peptide Antagonists for the Human Neurokinin-3 Receptor. 1. Identification of the 4-Quinolinecarboxamide Framework

AU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; Luttmann, Mark; et al.

CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy

SO J. Med. Chem. (1997), 40(12), 1794-1807
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CJACS-IMAGE; CJACS

AB A novel class of potent and selective non-peptide neurokinin-3 (NK-3) receptor antagonists, featuring the 4-quinolinecarboxamide framework, was designed based upon chem. diverse NK-1 receptor antagonists. The novel compds., prompted by chem. modifications of the prototype, were characterized by binding anal. using a membrane prepn. of chinese hamster ovary (CHO) cells expressing the human neurokinin-3 receptors (hNK-3-CHO), and clear structure-activity relationships (SARs) were established. From SARs, (R)-N-[α-(methoxycarbonyl)benzyl]-2-phenylquinoline-4-carboxamide (I, SB 218795, hNK-3-CHO binding K_i = 13 nM) emerged as one of the most potent compds. of this novel class. Selectivity studies vs. the other neurokinin receptors (hNK-2-CHO and hNK-1-CHO) revealed that 65 is about 90-fold selective for hNK-3 vs. hNK-2 receptors (hNK-2-CHO binding K_i = 1221 nM) and over 7000-fold selective vs. hNK-1 receptors (hNK-1-CHO binding K_i = >100 μM). In vitro functional studies in rabbit isolated iris sphincter muscle prepn. demonstrated that I a competitive antagonist of the contractile response induced by the potent and selective NK-3 receptor agonist senktide with a K_b = 43 nM. Overall, the data indicate that I is a potent and selective hNK-3 receptor antagonist and a useful lead for further chem. optimization.

IT ***174635-51-9P*** ***174635-52-0P*** ***174635-53-1P*** , SB 218795 ***174635-54-2P*** ***174635-56-4P*** ***174635-58-6P*** ***174635-59-7P*** ***174635-60-0P*** ***174635-61-1P*** ***174635-71-3P*** ***174635-73-5P*** ***174635-91-7P*** ***174635-97-3P*** ***174635-98-4P*** ***174636-00-1P*** ***174636-01-2P*** ***174636-04-5P*** ***174636-06-7P*** ***174636-07-8P*** ***174636-09-0P*** ***174636-13-6P*** ***174636-23-8P*** ***174636-24-9P*** ***174636-25-0P*** ***174636-40-9P*** ***189815-88-1P*** ***189815-93-8P*** ***189815-94-9P***

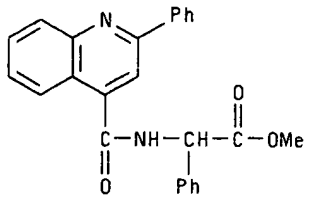
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of quinolinecarboxamide-contg. nonpeptide neurokinin-3 receptor antagonists)

RN 174635-51-9 CA

RN 174635-51-9 CA

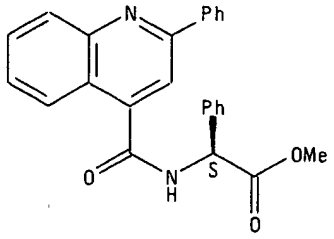
CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-52-0 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*S*)- (9CI) (CA INDEX NAME)

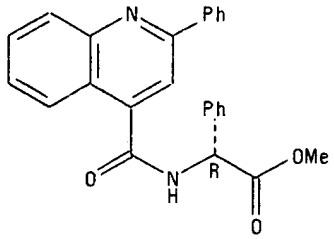
Absolute stereochemistry. Rotation (+).



RN 174635-53-1 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

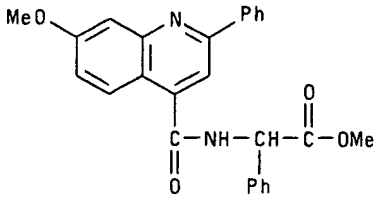
Absolute stereochemistry. Rotation (-).



RN 174635-54-2 CA

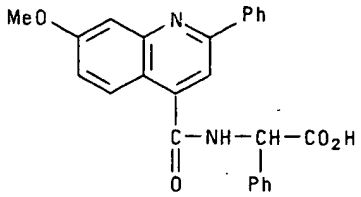
CN Benzeneacetic acid, α-[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-54-2 CA



RN 174635-56-4 CA

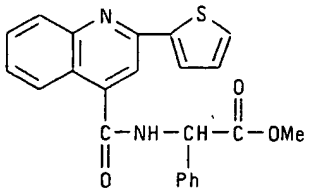
CN Benzeneacetic acid, α-[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



• HCl

RN 174635-58-6 CA

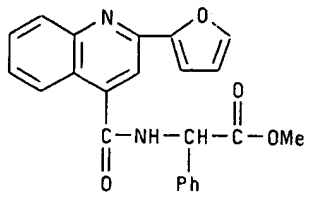
CN Benzeneacetic acid, α-[[[2-(2-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-59-7 CA

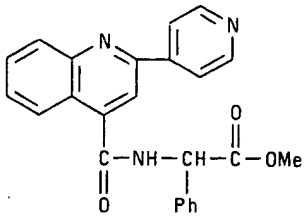
CN Benzeneacetic acid, α-[[[2-(2-furanyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-59-7 CA



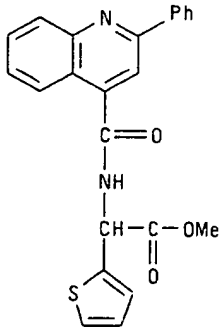
RN 174635-60-0 CA

CN Benzeneacetic acid, α-[[[2-(4-pyridinyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-61-1 CA

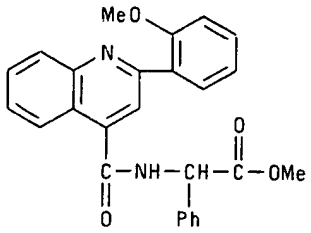
CN 2-Thiopheneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-71-3 CA

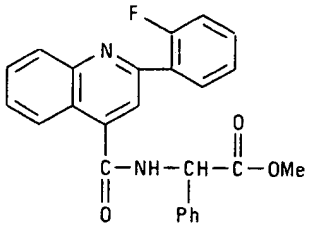
CN Benzeneacetic acid, α-[[[2-(2-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-71-3 CA



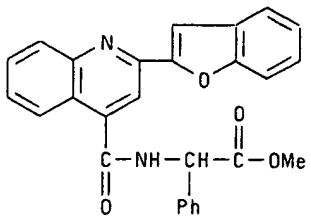
RN 174635-73-5 CA

CN Benzeneacetic acid, α-[[[2-(2-fluorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-91-7 CA

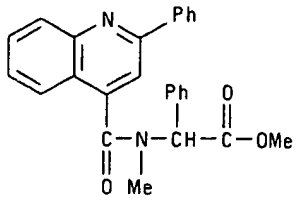
CN Benzeneacetic acid, α-[[[2-(2-benzofuranyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-97-3 CA

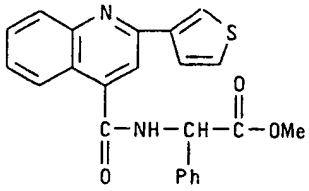
CN Benzeneacetic acid, α-[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-97-3 CA



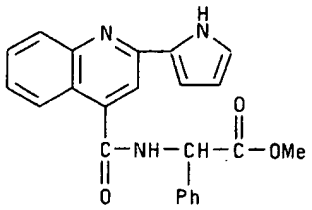
RN 174635-98-4 CA

CN Benzeneacetic acid, α-[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



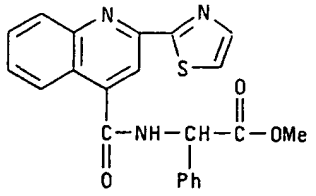
RN 174636-00-1 CA

CN Benzeneacetic acid, α-[[[2-(1*H*-pyrrol-2-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-01-2 CA

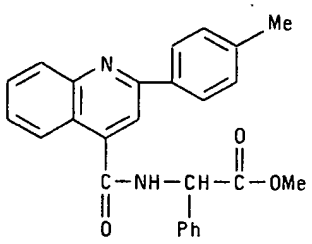
CN Benzeneacetic acid, α-[[[2-(2-thiazolyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-04-5 CA

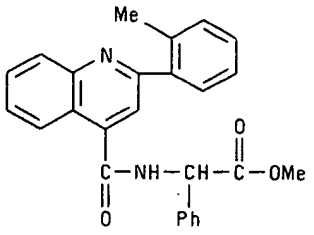
RN 174636-04-5 CA

CN Benzeneacetic acid, α-[[[2-(4-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



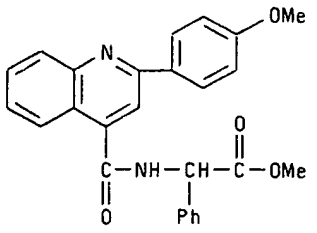
RN 174636-06-7 CA

CN Benzeneacetic acid, α-[[[2-(2-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-07-8 CA

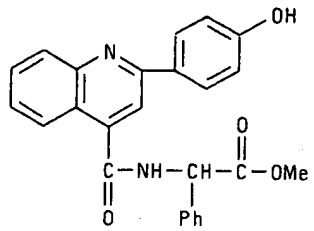
CN Benzeneacetic acid, α-[[[2-(4-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-09-0 CA

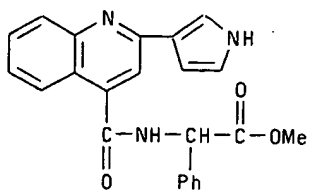
CN Benzeneacetic acid, α-[[[2-(4-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-09-0 CA



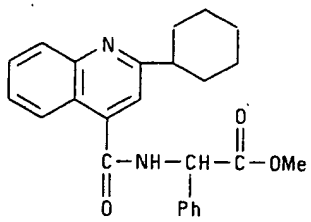
RN 174636-13-6 CA

CN Benzeneacetic acid, α-[[[2-(1*H*-pyrrol-3-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



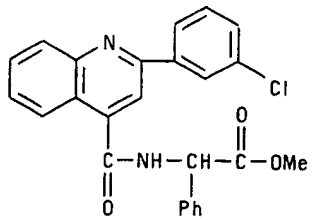
RN 174636-23-8 CA

CN Benzeneacetic acid, α-[[(2-cyclohexyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-24-9 CA

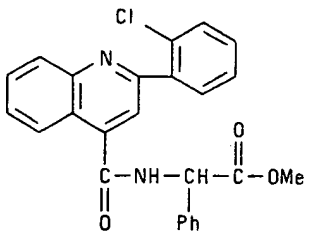
CN Benzeneacetic acid, α-[[[2-(3-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-24-9 CA

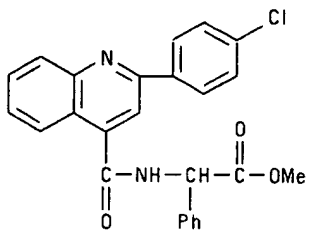
RN 174636-25-0 CA

CN Benzeneacetic acid, α-[[[2-(2-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



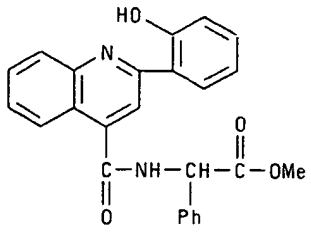
RN 174636-40-9 CA

CN Benzeneacetic acid, α-[[[2-(4-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 189815-88-1 CA

CN Benzeneacetic acid, α-[[[2-(2-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

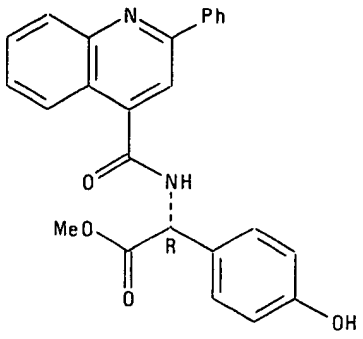


RN 189815-93-8 CA

CN Benzeneacetic acid, 4-hydroxy-α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

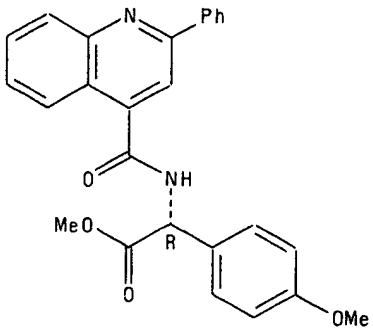
RN 189815-93-8 CA



RN 189815-94-9 CA

CN Benzeneacetic acid, 4-methoxy-α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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DUPLICATE 6

L6 ANSWER 6 OF 17 CA COPYRIGHT 1997 ACS

AN 127:104218 CA

TI Nonpeptide tachykinin receptor antagonists: I. Pharmacological and pharmacokinetic characterization of SB 223412, a novel, potent and selective neurokinin-3 receptor antagonist

AU Sarau, Henry M.; Griswold, Don E.; Potts, William; Foley, James J.; Schmidt, Dulcie B.; Webb, Edward F.; Martin, Lenox D.; Brawner, Mary E.; Elshourbagy, Nabil A.; Medhurst, Andrew D.; Giardina, Giuseppe A. M.; Hay, Douglas W. P.

CS Departments of Pulmonary Pharmacology, Immunopharmacology, Drug Metabolism and Pharmacokinetics, Gene Expression Sciences and Molecular Genetics, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406, USA

SO J. Pharmacol. Exp. Ther. (1997), 281(3), 1303-1311
CODEN: JPETAB; ISSN: 0022-3565

PB Williams & Wilkins

DT Journal

LA English

AB The in vitro and in vivo pharmacol. profile of SB 223412 [(S)-(-)-N-(α-ethylbenzyl)-3-hydroxy-2-phenylquinoline-4-carboxamide], a novel human NK-3 (hNK-3) receptor antagonist, is described. SB 223412 demonstrated enantioselective affinity for inhibition of [^{125}I][MePhe^{7}]neurokinin B (NKB) binding to membranes of CHO cells expressing the hNK-3 receptor (CHO hNK-3). SB 223412, the (S)-isomer, (K_i = 1.0 nM), has similar affinity as the natural ligand, NKB (K_i = 0.8 nM) and another nonpeptide NK-3 receptor antagonist, SR 142801 (K_i = 1.2 nM). SB 223412 was selective for hNK-3 receptors compared with hNK-1 (>10,000-fold selective) and hNK-2 receptors (>140-fold selective), and selectivity was further demonstrated by its lack of effect, in concns. up to 1 or 10 μM, in >60 receptor, enzyme and ion channel assays. SB 223412 enantioselectively inhibited the NKB-induced Ca^{++} mobilization in HEK 293 cells stably expressing the hNK-3 receptor. SB 223412 (10-1,000 nM) produced concn.-dependent rightward shifts in NKB-induced CA^{++} mobilization concn.-response curves with a K_b value of 3 nM. In addn., SB 223412 antagonized senktide-induced contraction in the isolated rabbit iris sphincter muscle (K_b = 1.6 nM). In mice, oral administration of SB 223412 produced dose-dependent inhibition of behavioral responses induced by the NK-3 receptor-selective agonist, senktide (ED_{50} = 12.2 mg/kg). Pharmacokinetic evaluation of SB 223412 in rat and dog indicted low plasma clearance, oral bioavailability and high and sustained plasma concns. after 4 to 8 mg/kg oral dosages. The preclin. profile of SB 223412 (high affinity, selectivity, reversibility and oral activity) suggests that it will be a useful tool compd. to define the physiol. and pathophysiol. roles of NK-3 receptors.

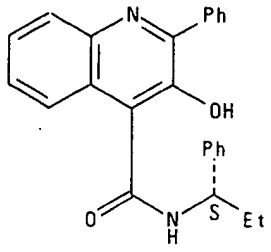
IT ***174636-32-9*** , SB 223412
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL (Biological study); PROC (Process)
(pharmacol. and pharmacokinetic characterization of NK-3 antagonist SB 223412)

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX

RN 174636-32-9 CA

Absolute stereochemistry. Rotation (-).



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L6 ANSWER 7 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 7

AN 127:4735 CA

TI Direct tritium labeling of multifunctional compounds using organoiridium catalysis

AU Chen, W.; Garnes, K.T.; Levinson, S.H.; Saunders, D.; Senderoff, S.G.; Shu, A.Y.L.; Villani, A.J.; Heys, J.R.

CS Radiochemistry, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406, USA

SO J. Labelled Compd. Radiopharm. (1997), 39(4), 291-298
CODEN: JLCRD4; ISSN: 0362-4803

PB Wiley

DT Journal

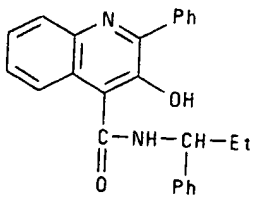
LA English

AB The tritium exchange labeling of a variety of complex compds. is achieved in the presence of catalyst precursor $[(cod)Ir(PPh_3)_2]BF_4$ and limited amts. of tritium gas. The regioselectivity of exchange is high and consistent with empirical rules previously obsd. High specific activity levels are often achieved, usually with specific aryl C-H bonds. However, remarkably efficient exchange occurs in certain N-alkyl groups. Studies of intermol. inhibition of catalytic exchange suggest reasons why larger amts. of complex are sometimes required to label complex mols.; nevertheless, significant amts. of label incorporation into substrates can be achieved even starting with small amts. of labeling gas.

IT ***174636-26-1DP*** , deuterated
RL: SPN (Synthetic preparation); PREP (Preparation)
(direct deuterium labeling of multifunctional compds. using organoiridium catalysts)

RN 174636-26-1 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

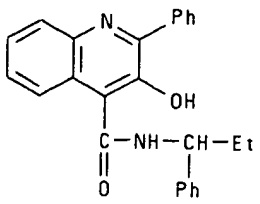


IT ***174636-26-1***
RL: RCT (Reactant)
(direct tritium labeling of multifunctional compds. using organoiridium catalysts)

RN 174636-26-1 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

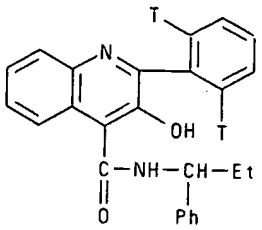
RN 174636-26-1 CA



IT ***190187-74-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(direct tritium labeling of multifunctional compds. using organoiridium catalysts)

RN 190187-74-7 CA

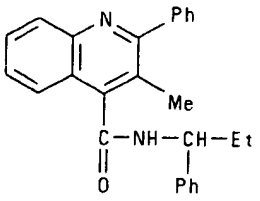
CN 4-Quinolinecarboxamide, 3-hydroxy-2-(phenyl-*2,6-t*$_2$)-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



IT ***174635-78-0***
RL: RCT (Reactant)
(inhibition of Et benzoate deuteration by dioxa compds.)

RN 174635-78-0 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



IT ***174635-78-0DP*** , deuterated
RL: SPN (Synthetic preparation); PREP (Preparation)
(inhibition of Et benzoate deuteration by dioxa compds.)

RN 174635-78-0 CA

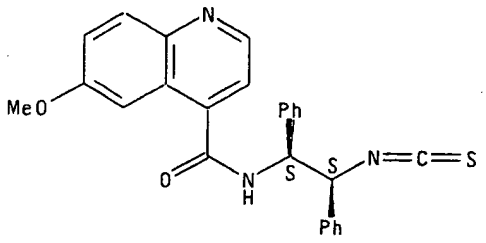
CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 185508-92-3 CA

RN 185508-92-3 CA

CN 4-Quinolinecarboxamide, *N*-(2-isothiocyanato-1,2-diphenylethyl)-6-methoxy-, [*S*-(*R**,*R**)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L6 ANSWER 9 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 9

AN 125:25636 CA

TI 2-Phenyl-4-quinolinecarboxamides: A Novel Class of Potent and Selective Non-Peptide Competitive Antagonists for the Human Neurokinin-3 Receptor

AU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Foley, James J.; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; et al.

CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy

SO J. Med. Chem. (1996), 39(12), 2281-2284
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CJACS-IMAGE; CJACS

AB A novel class of potent and selective, non-peptide NK-3 receptor antagonists, based on the 2-phenylquinoline framework, has been identified and characterized by binding anal. using membrane prepn. of CHO cells expressing the human neurokinin receptors (hNKs-CHO). Functional activity was detd. by inhibition of senktide-induced contraction of the rabbit isolated iris sphincter muscle prepn. An extensive structure-activity study led to the identification of (S)-(-)-N-(α-ethylbenzyl)-3-hydroxy-2-phenylquinoline-4-carboxamide (SB 223412) as the most potent (K_i = 1.0 nm in hNK-3-CHO binding; K_b = 5.4 nM for antagonism of senktide-induced contraction in rabbit iris sphincter muscle) and selective (hNK-2/hNK-3 K_i ratio of 144 and hNK-1/hNK-3 K_i ratio > 100,000) hNK-3 receptor antagonist of this class. In addn., NKB-induced Ca^{2+} mobilization studies in hNK-3-HEK 293 cells indicated that SB 223412 is a reversible, competitive antagonist. Compds. from this novel class will be extremely useful in the functional characterization of hNK-3 receptors and elucidation of potential therapeutic indications for selective hNK-3 receptor antagonists.

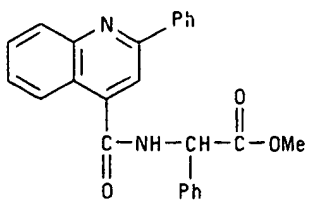
IT ***174635-51-9P*** ***174635-52-0P*** ***174635-53-1P*** ***174635-69-9P*** ***174636-20-5P*** ***174636-32-9P*** , SB 223412

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and structure-activity of human neurokinin 3 receptor antagonists phenylquinolinecarboxamides)

RN 174635-51-9 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

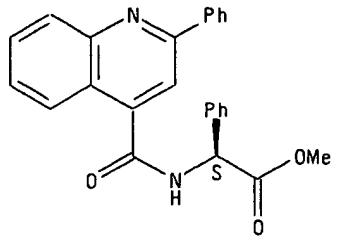


RN 174635-52-0 CA

RN 174635-52-0 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*S*)- (9CI) (CA INDEX NAME)

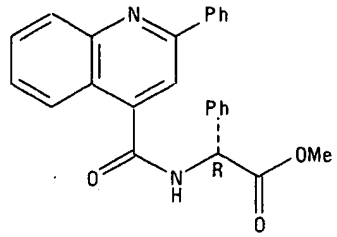
Absolute stereochemistry. Rotation (+).



RN 174635-53-1 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

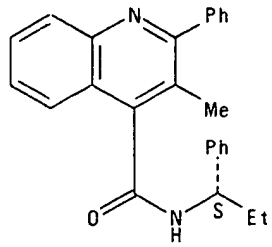
Absolute stereochemistry. Rotation (-).



RN 174635-69-9 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

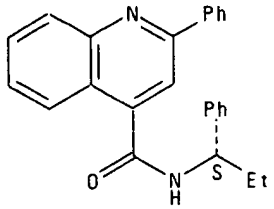


RN 174636-20-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

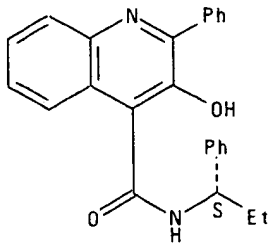
RN 174636-20-5 CA



RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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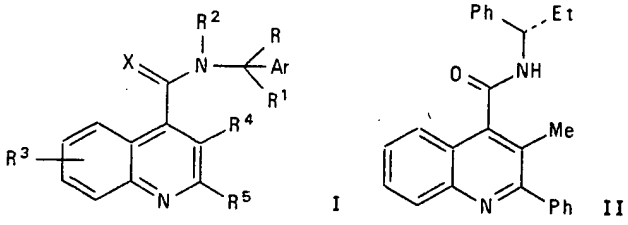
L6 ANSWER 10 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 10
AN 124:232269 CA
TI Quinoline derivatives as tachykinin NK_3 receptor antagonists
IN Farina, Carlo; Giardina, Giuseppe Arnaldo Mari; Grugni, Mario; Raveglia, Luca Francesco
PA Smithkline Beecham Farmaceutici S.P.A., Italy
SO PCT Int. Appl., 95 pp.
CODEN: PIXXD2
PI WO 9532948 A1 951207
DS W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI WO 95-EP2000 950523
PRAI IT 94-MI1099 940527
IT 95-MI494 950314
DT Patent
LA English
OS MARPAT 124:232269
GI



AB NK_3 receptor antagonists **I** [Ar = (un)substituted Ph, naphthyl, cycloalkadienyl, heteroaryl; R = (un)substituted alkyl, cycloalkyl, (un)substituted Ph, phenylalkyl, or heteroaryl, CO_2H and derivs., etc.; R^1, R^2 = H, alkyl; or R^1R^2 = $(CH_2)_{3-5}$; or RR^1 = $(CH_2)_{2-5}$; R^3, R^4 = H, alkyl, alkenyl, aryl, alkoxy, OH, halo, NO_2, amino, etc.; R^5 = alkyl, cycloalkyl, (un)substituted (hetero)aryl; X = O, S, N(CN)] are useful in treating pulmonary, CNS, and neurodegenerative disorders, etc. Approx. 115 compds. were prepd. For example, amidation of 3-methyl-2-phenylquinoline-4-carbonyl chloride with (R)-α-ethylbenzylamine gave title compd. **II** in 58% yield. **II** had IC_{50} of 5.6 nM for displacement of [^{3}H]-senktide from guinea-pig cortical NK_3 receptors. Antagonist activity of **I** was shown by inhibition of senktide-induced contraction of guinea-pig ileum.

IT ***174635-48-4P*** ***174635-49-5P*** ***174635-50-8P*** ***174635-51-9P*** ***174635-52-0P*** ***174635-53-1P*** ***174635-54-2P***

L6 ANSWER 10 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 10

174635-55-3P ***174635-56-4P*** ***174635-57-5P*** ***174635-58-6P*** ***174635-59-7P*** ***174635-60-0P*** ***174635-61-1P*** ***174635-62-2P*** ***174635-63-3P*** ***174635-64-4P*** ***174635-65-5P*** ***174635-66-6P*** ***174635-68-8P*** ***174635-69-9P*** ***174635-70-2P*** ***174635-71-3P*** ***174635-72-4P*** ***174635-73-5P*** ***174635-74-6P*** ***174635-75-7P*** ***174635-76-8P*** ***174635-77-9P*** ***174635-78-0P*** ***174635-79-1P*** ***174635-80-4P*** ***174635-81-5P*** ***174635-82-6P*** ***174635-83-7P*** ***174635-84-8P*** ***174635-85-9P*** ***174635-86-0P*** ***174635-87-1P*** ***174635-88-2P*** ***174635-89-3P*** ***174635-90-6P*** ***174635-91-7P*** ***174635-92-8P*** ***174635-93-9P*** ***174635-94-0P*** ***174635-95-1P*** ***174635-96-2P*** ***174635-97-3P*** ***174635-98-4P*** ***174636-00-1P*** ***174636-01-2P*** ***174636-03-4P*** ***174636-04-5P*** ***174636-05-6P*** ***174636-06-7P*** ***174636-07-8P*** ***174636-09-0P*** ***174636-10-3P*** ***174636-11-4P*** ***174636-12-5P*** ***174636-13-6P*** ***174636-14-7P*** ***174636-15-8P*** ***174636-16-9P*** ***174636-17-0P*** ***174636-18-1P*** ***174636-19-2P*** ***174636-20-5P*** ***174636-21-6P*** ***174636-22-7P*** ***174636-23-8P*** ***174636-24-9P*** ***174636-25-0P*** ***174636-26-1P*** ***174636-27-2P*** ***174636-28-3P*** ***174636-29-4P*** ***174636-30-7P*** ***174636-31-8P*** ***174636-32-9P*** ***174636-33-0P*** ***174636-34-1P*** ***174636-35-2P*** ***174636-36-3P*** ***174636-37-4P*** ***174636-38-5P*** ***174636-39-6P*** ***174636-40-9P*** ***174636-41-0P*** ***174636-42-1P*** ***174636-43-2P*** ***174636-44-3P*** ***174636-45-4P*** ***174636-46-5P*** ***174636-47-6P*** ***174636-48-7P*** ***174636-49-8P*** ***174636-50-1P*** ***174636-51-2P*** ***174636-52-3P*** ***174636-53-4P*** ***174636-54-5P*** ***174636-55-6P*** ***174636-56-7P*** ***174636-57-8P*** ***174636-58-9P*** ***174636-59-0P*** ***174636-60-3P*** ***174636-61-4P*** ***174636-62-5P***

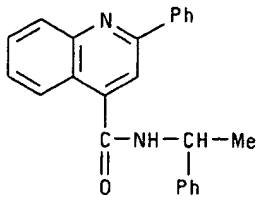
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinolinecarboxamide derivs. as tachykinin NK_3 receptor antagonists)

RN 174635-48-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylethyl)- (9CI) (CA INDEX NAME)

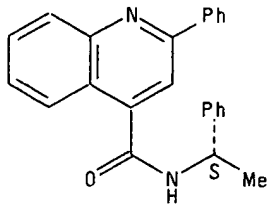
RN 174635-48-4 CA



RN 174635-49-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylethyl)-, (*S*)- (9CI) (CA INDEX NAME)

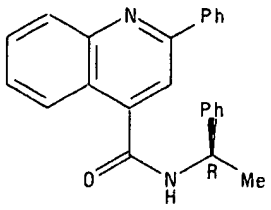
Absolute stereochemistry. Rotation (+).



RN 174635-50-8 CA

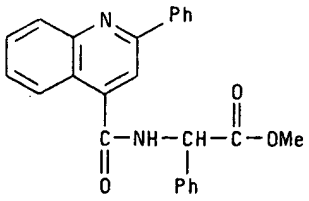
CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylethyl)-, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 174635-51-9 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

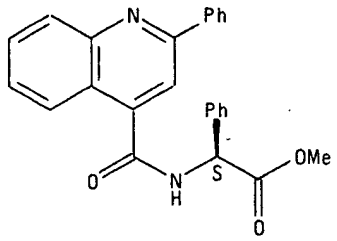


RN 174635-52-0 CA

RN 174635-52-0 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*S*)- (9CI) (CA INDEX NAME)

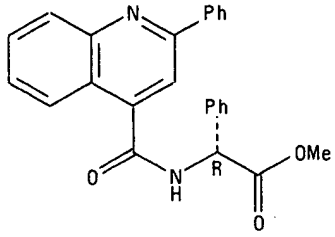
Absolute stereochemistry. Rotation (+).



RN 174635-53-1 CA

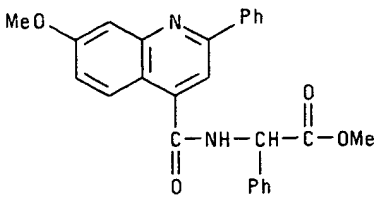
CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 174635-54-2 CA

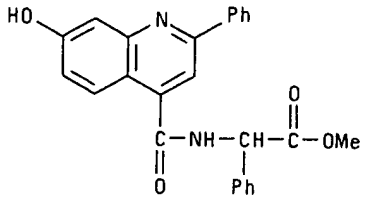
CN Benzeneacetic acid, α-[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-55-3 CA

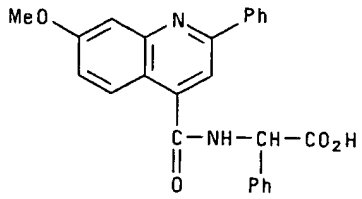
CN Benzeneacetic acid, α-[[(7-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-55-3 CA



RN 174635-56-4 CA

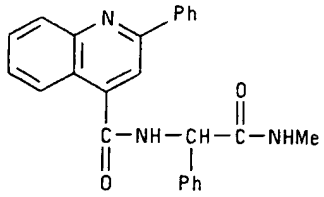
CN Benzeneacetic acid, α-[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



• HCl

RN 174635-57-5 CA

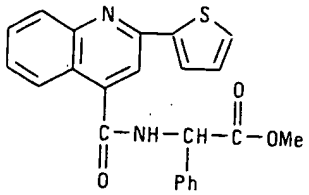
CN 4-Quinolinecarboxamide, N-[2-(methylamino)-2-oxo-1-phenylethyl]-2-phenyl- (9CI) (CA INDEX NAME)



RN 174635-58-6 CA

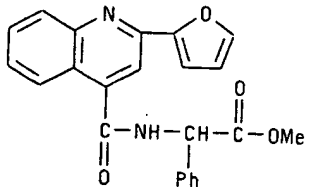
CN Benzeneacetic acid, α-[[[2-(2-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-58-6 CA



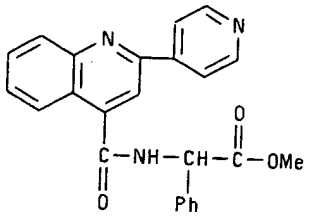
RN 174635-59-7 CA

CN Benzeneacetic acid, α-[[[2-(2-furanyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-60-0 CA

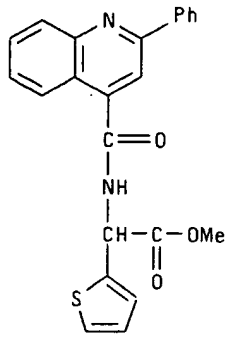
CN Benzeneacetic acid, α-[[[2-(4-pyridinyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-61-1 CA

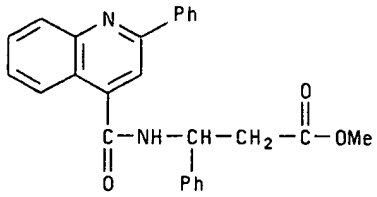
CN 2-Thiopheneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-61-1 CA



RN 174635-62-2 CA

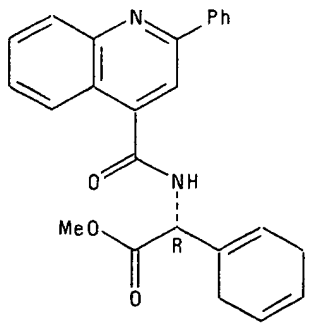
CN Benzenepropanoic acid, β-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-63-3 CA

CN 1,4-Cyclohexadiene-1-acetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

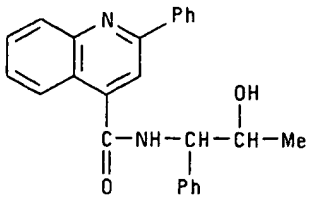
Absolute stereochemistry. Rotation (-).



RN 174635-64-4 CA

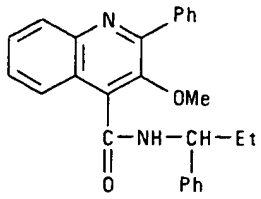
CN 4-Quinolinecarboxamide, *N*-(2-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME).

RN 174635-64-4 CA



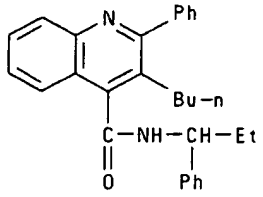
RN 174635-65-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



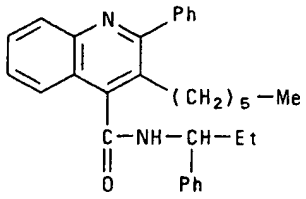
RN 174635-66-6 CA

CN 4-Quinolinecarboxamide, 3-butyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



RN 174635-68-8 CA

CN 4-Quinolinecarboxamide, 3-hexyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

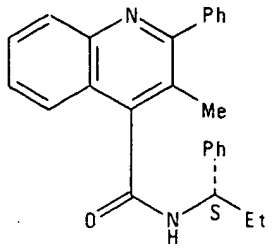


RN 174635-69-9 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

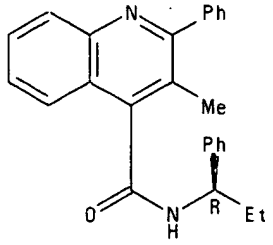
RN 174635-69-9 CA



RN 174635-70-2 CA

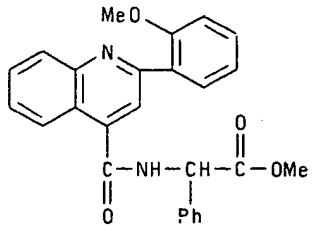
CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 174635-71-3 CA

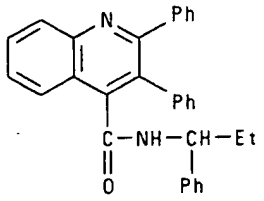
CN Benzeneacetic acid, α-[[[2-(2-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-72-4 CA

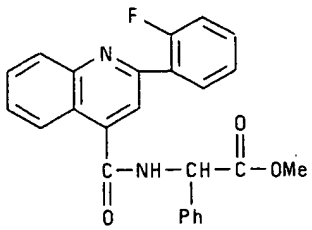
CN 4-Quinolinecarboxamide, 2,3-diphenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-72-4 CA



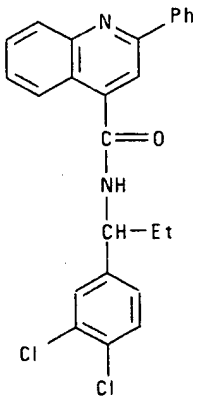
RN 174635-73-5 CA

CN Benzeneacetic acid, α-[[[2-(2-fluorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-74-6 CA

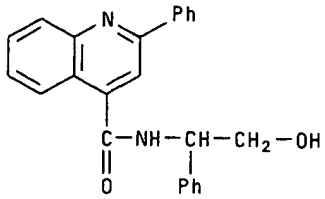
CN 4-Quinolinecarboxamide, *N*-[1-(3,4-dichlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)



RN 174635-75-7 CA

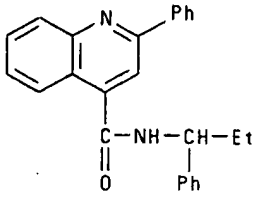
CN 4-Quinolinecarboxamide, *N*-(2-hydroxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-75-7 CA



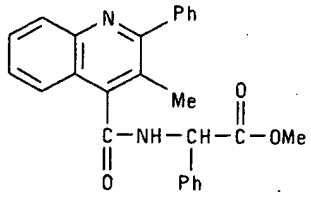
RN 174635-76-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



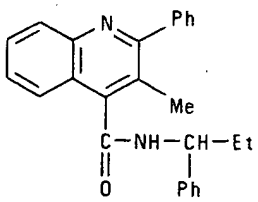
RN 174635-77-9 CA

CN Benzeneacetic acid, α-[[(3-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-78-0 CA

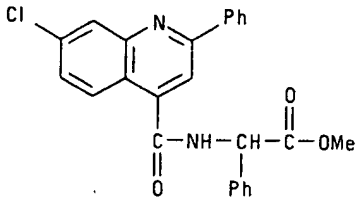
CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



RN 174635-79-1 CA

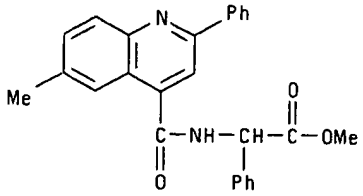
RN 174635-79-1 CA

CN Benzeneacetic acid, α-[[(7-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



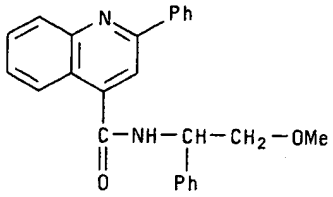
RN 174635-80-4 CA

CN Benzeneacetic acid, α-[[(6-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



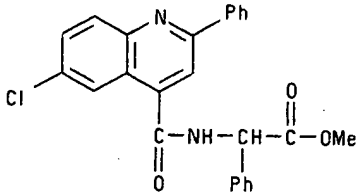
RN 174635-81-5 CA

CN 4-Quinolinecarboxamide, *N*-(2-methoxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174635-82-6 CA

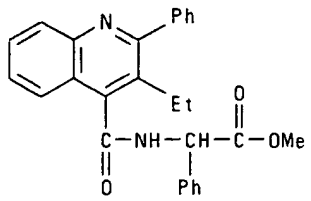
CN Benzeneacetic acid, α-[[(6-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-82-6 CA

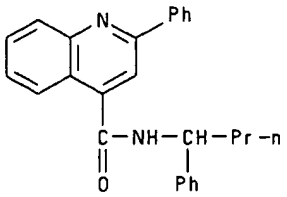
RN 174635-83-7 CA

CN Benzeneacetic acid, α-[[(3-ethyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



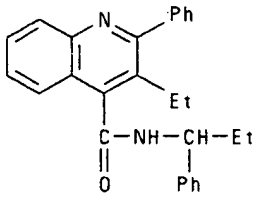
RN 174635-84-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylbutyl)- (9CI) (CA INDEX NAME)



RN 174635-85-9 CA

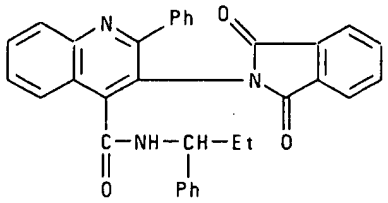
CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



RN 174635-86-0 CA

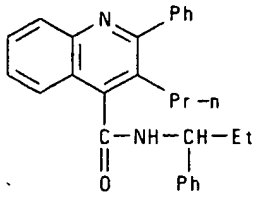
CN 4-Quinolinecarboxamide, 3-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-86-0 CA



RN 174635-87-1 CA

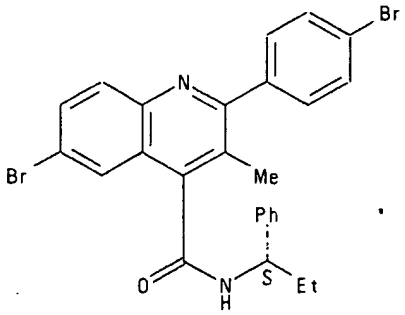
CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-propyl- (9CI) (CA INDEX NAME)



RN 174635-88-2 CA

CN 4-Quinolinecarboxamide, 6-bromo-2-(4-bromophenyl)-3-methyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

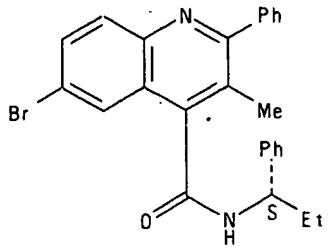


RN 174635-89-3 CA

CN 4-Quinolinecarboxamide, 6-bromo-3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

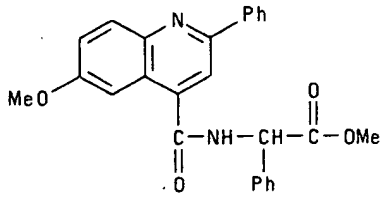
Absolute stereochemistry. Rotation (-).

RN 174635-89-3 CA



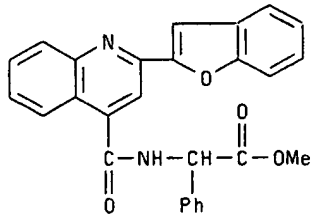
RN 174635-90-6 CA

CN Benzeneacetic acid, α-[[(6-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



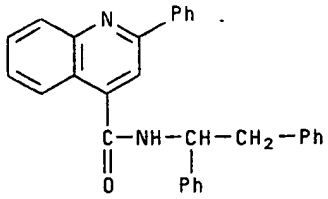
RN 174635-91-7 CA

CN Benzeneacetic acid, α-[[[2-(2-benzofuranyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-92-8 CA

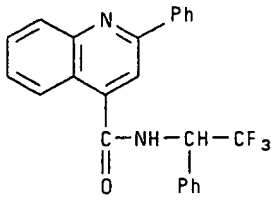
CN 4-Quinolinecarboxamide, *N*-(1,2-diphenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174635-93-9 CA

RN 174635-93-9 CA

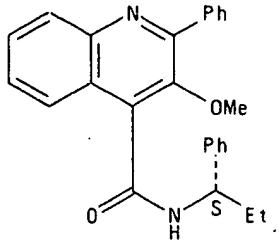
CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(2,2,2-trifluoro-1-phenylethyl)- (9CI) (CA INDEX NAME)



RN 174635-94-0 CA

CN 4-Quinolinecarboxamide, 3-methoxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

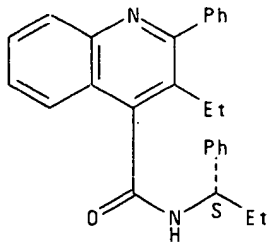
Absolute stereochemistry. Rotation (-).



RN 174635-95-1 CA

CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

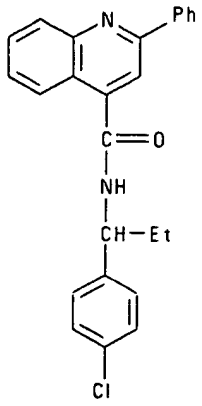
Absolute stereochemistry. Rotation (-).



RN 174635-96-2 CA

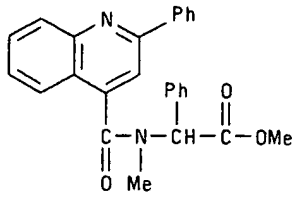
CN 4-Quinolinecarboxamide, *N*-[1-(4-chlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-96-2 CA



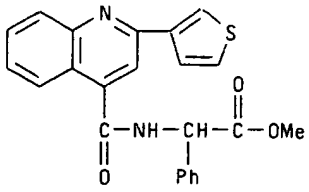
RN 174635-97-3 CA

CN Benzeneacetic acid, α-[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174635-98-4 CA

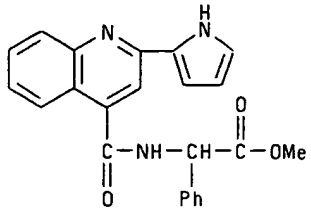
CN Benzeneacetic acid, α-[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-00-1 CA

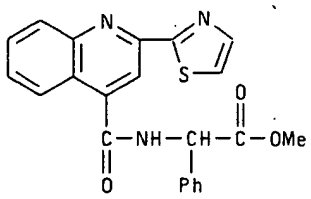
CN Benzeneacetic acid, α-[[[2-(1*H*-pyrrol-2-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-00-1 CA



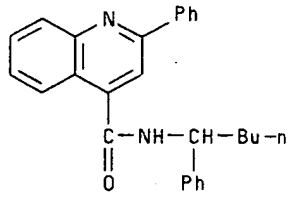
RN 174636-01-2 CA

CN Benzeneacetic acid, α-[[[2-(2-thiazolyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



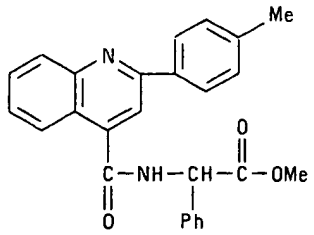
RN 174636-03-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpentyl)- (9CI) (CA INDEX NAME)



RN 174636-04-5 CA

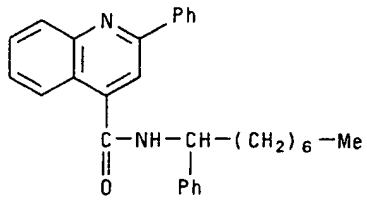
CN Benzeneacetic acid, α-[[[2-(4-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-05-6 CA

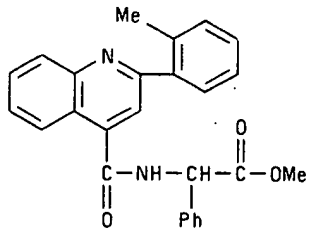
RN 174636-05-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenyloctyl)- (9CI) (CA INDEX NAME)



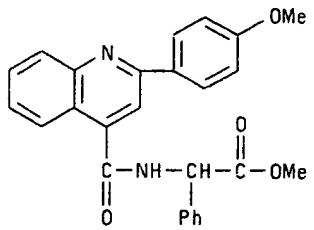
RN 174636-06-7 CA

CN Benzeneacetic acid, α-[[[2-(2-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-07-8 CA

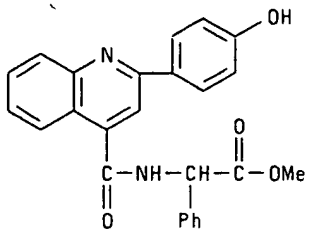
CN Benzeneacetic acid, α-[[[2-(4-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-09-0 CA

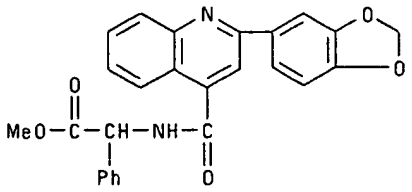
CN Benzeneacetic acid, α-[[[2-(4-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-09-0 CA



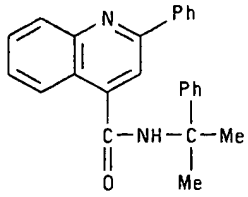
RN 174636-10-3 CA

CN Benzeneacetic acid, α-[[[2-(1,3-benzodioxol-5-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-11-4 CA

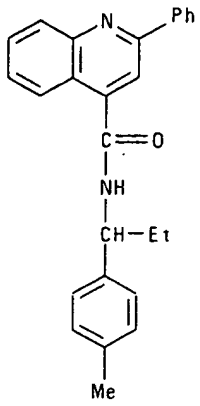
CN 4-Quinolinecarboxamide, *N*-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-12-5 CA

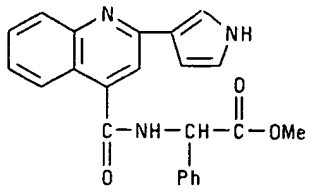
CN 4-Quinolinecarboxamide, *N*-[1-(4-methylphenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-12-5 CA



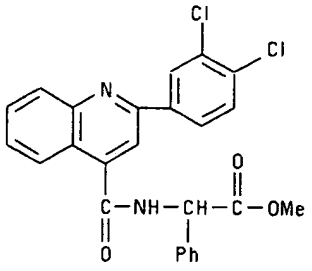
RN 174636-13-6 CA

CN Benzeneacetic acid, α-[[[2-(1*H*-pyrrol-3-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-14-7 CA

CN Benzeneacetic acid, α-[[[2-(3,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

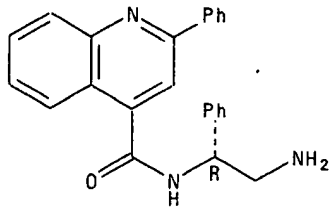


RN 174636-15-8 CA

CN 4-Quinolinecarboxamide, *N*-(2-amino-1-phenylethyl)-2-phenyl-, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

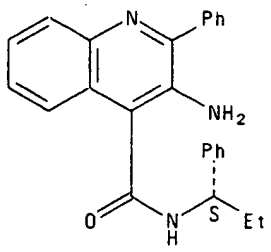
RN 174636-15-8 CA



RN 174636-16-9 CA

CN 4-Quinolinecarboxamide, 3-amino-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

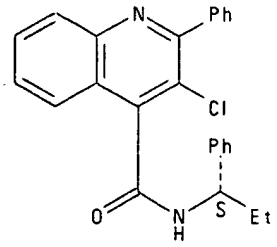
Absolute stereochemistry. Rotation (-).



RN 174636-17-0 CA

CN 4-Quinolinecarboxamide, 3-chloro-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

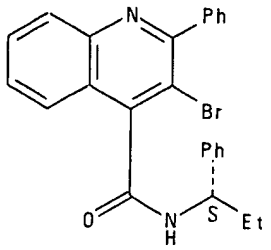


RN 174636-18-1 CA

CN 4-Quinolinecarboxamide, 3-bromo-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

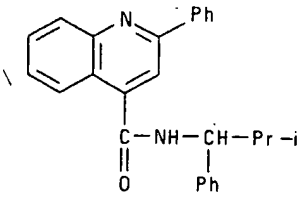
Absolute stereochemistry. Rotation (-).

RN 174636-18-1 CA



RN 174636-19-2 CA

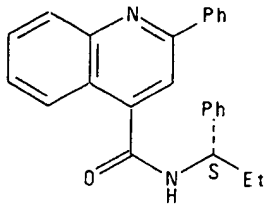
CN 4-Quinolinecarboxamide, *N*-(2-methyl-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-20-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

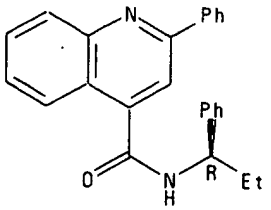
Absolute stereochemistry. Rotation (-).



RN 174636-21-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-, (*R*)- (9CI) (CA INDEX NAME)

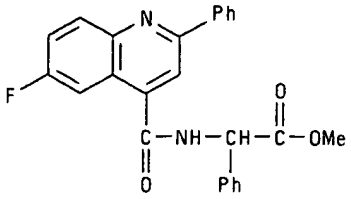
Absolute stereochemistry. Rotation (+).



RN 174636-22-7 CA

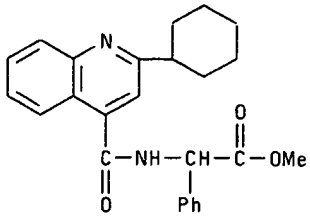
RN 174636-22-7 CA

CN Benzeneacetic acid, α-[[(6-fluoro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



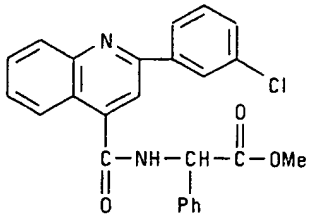
RN 174636-23-8 CA

CN Benzeneacetic acid, α-[[(2-cyclohexyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-24-9 CA

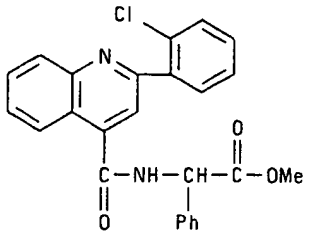
CN Benzeneacetic acid, α-[[[2-(3-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-25-0 CA

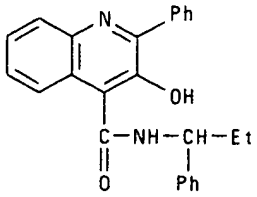
CN Benzeneacetic acid, α-[[[2-(2-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-25-0 CA



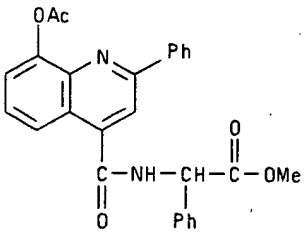
RN 174636-26-1 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)- (9CI) (CA INDEX NAME)



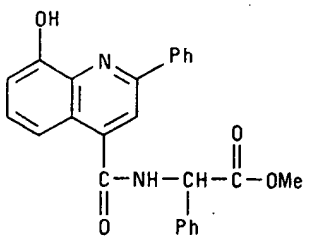
RN 174636-27-2 CA

CN Benzeneacetic acid, α-[[[8-(acetyloxy)-2-phenyl-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-28-3 CA

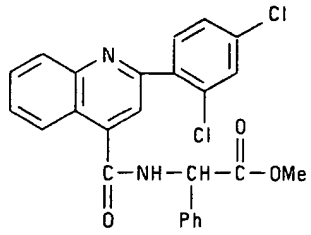
CN Benzeneacetic acid, α-[[(8-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-28-3 CA

RN 174636-29-4 CA

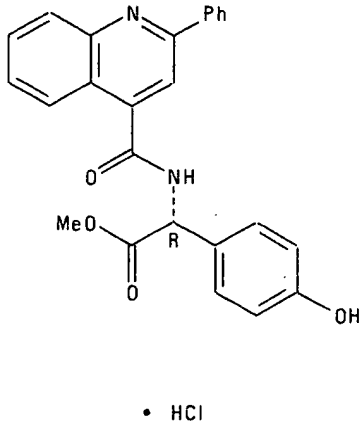
CN Benzeneacetic acid, α-[[[2-(2,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-30-7 CA

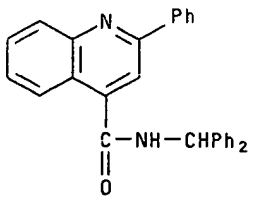
CN Benzeneacetic acid, 4-hydroxy-α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, monohydrochloride, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 174636-31-8 CA

CN 4-Quinolinecarboxamide, *N*-(diphenylmethyl)-2-phenyl- (9CI) (CA INDEX NAME)

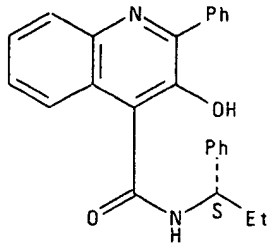


RN 174636-32-9 CA

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

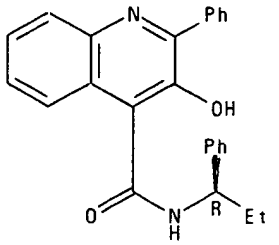
Absolute stereochemistry. Rotation (-).



RN 174636-33-0 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-*N*-(1-phenylpropyl)-, (*R*)- (9CI) (CA INDEX NAME)

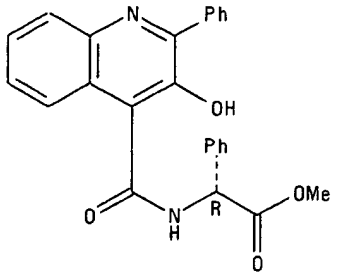
Absolute stereochemistry. Rotation (+).



RN 174636-34-1 CA

CN Benzeneacetic acid, α-[[(3-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (*R*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

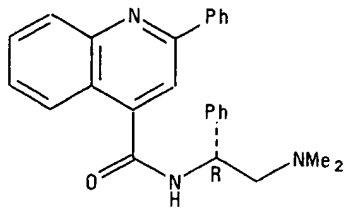


RN 174636-35-2 CA

CN 4-Quinolinecarboxamide, *N*-[2-(dimethylamino)-1-phenylethyl]-2-phenyl-, (*R*)- (9CI) (CA INDEX NAME)

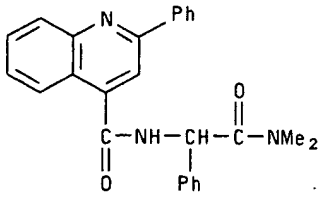
RN 174636-35-2 CA

Absolute stereochemistry. Rotation (-).



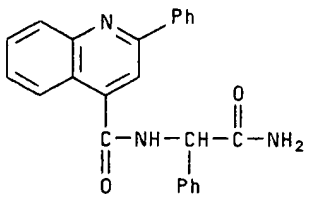
RN 174636-36-3 CA

CN 4-Quinolinecarboxamide, *N*-[2-(dimethylamino)-2-oxo-1-phenylethyl]-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-37-4 CA

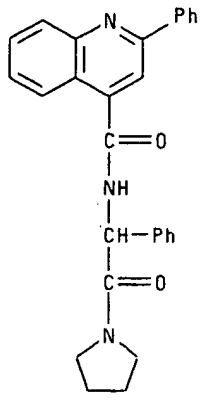
CN 4-Quinolinecarboxamide, *N*-(2-amino-2-oxo-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-38-5 CA

CN 4-Quinolinecarboxamide, *N*-[2-oxo-1-phenyl-2-(1-pyrrolidinyl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

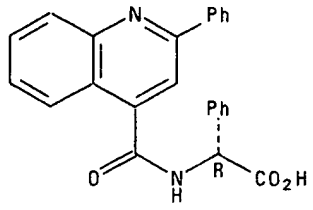
RN 174636-38-5 CA



RN 174636-39-6 CA

CN Benzeneacetic acid, α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride, (*R*)- (9CI) (CA INDEX NAME)

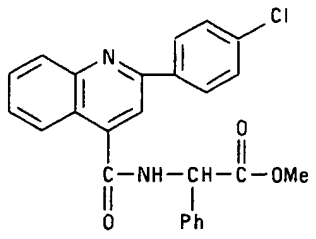
Absolute stereochemistry. Rotation (-).



• HCl

RN 174636-40-9 CA

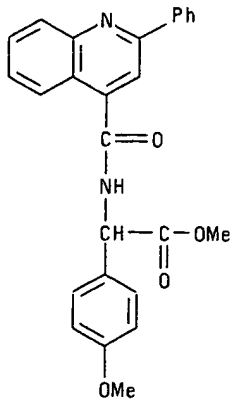
CN Benzeneacetic acid, α-[[[2-(4-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-41-0 CA

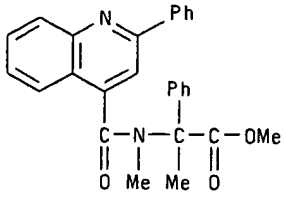
RN 174636-41-0 CA

CN Benzeneacetic acid, 4-methoxy-α-[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 174636-42-1 CA

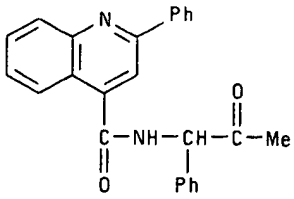
CN Benzeneacetic acid, α-methyl-α-[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



• HCl

RN 174636-43-2 CA

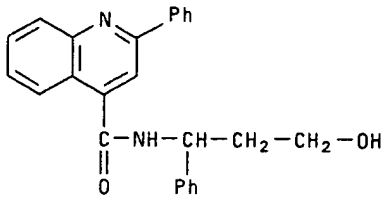
CN 4-Quinolinecarboxamide, N-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-44-3 CA

CN 4-Quinolinecarboxamide, N-(3-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

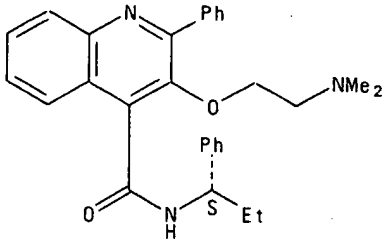
RN 174636-44-3 CA



RN 174636-45-4 CA

CN 4-Quinolinecarboxamide, 3-[2-(dimethylamino)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

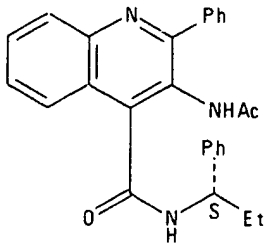


• HCl

RN 174636-46-5 CA

CN 4-Quinolinecarboxamide, 3-(acetylamino)-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

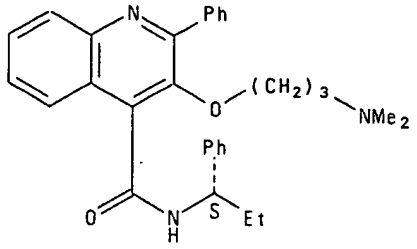


RN 174636-47-6 CA

CN 4-Quinolinecarboxamide, 3-[3-(dimethylamino)propoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174636-47-6 CA

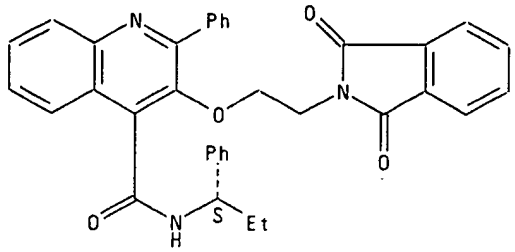


• HCl

RN 174636-48-7 CA

CN 4-Quinolinecarboxamide, 3-[2-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



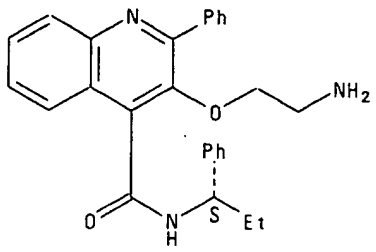
• HCl

RN 174636-49-8 CA

CN 4-Quinolinecarboxamide, 3-(2-aminoethoxy)-2-phenyl-*N*-(1-phenylpropyl)-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174636-49-8 CA

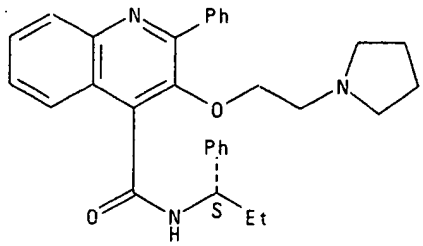


• HCl

RN 174636-50-1 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-(1-phenylpropyl)-3-[2-(1-pyrrolidinyl)ethoxy]-, monohydrochloride, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

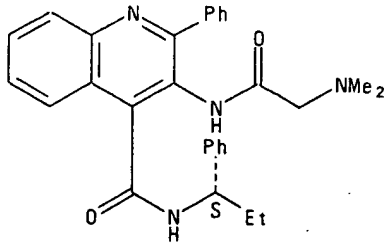


• HCl

RN 174636-51-2 CA

CN 4-Quinolinecarboxamide, 3-[[(dimethylamino)acetyl]amino]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

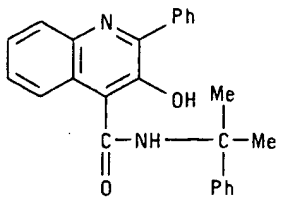
Absolute stereochemistry. Rotation (-).



RN 174636-52-3 CA

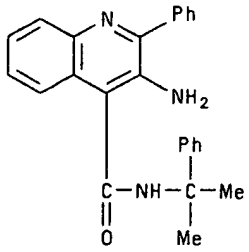
RN 174636-52-3 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-*N*-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



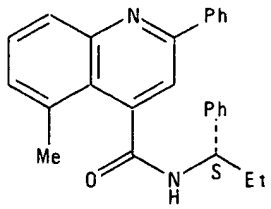
RN 174636-53-4 CA

CN 4-Quinolinecarboxamide, 3-amino-*N*-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-54-5 CA

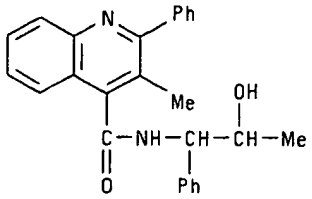
CN 4-Quinolinecarboxamide, 5-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)
Absolute stereochemistry. Rotation (-).



RN 174636-55-6 CA

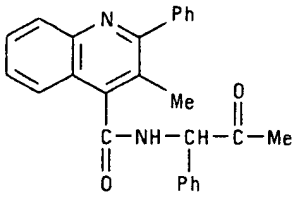
CN 4-Quinolinecarboxamide, *N*-(2-hydroxy-1-phenylpropyl)-3-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-55-6 CA



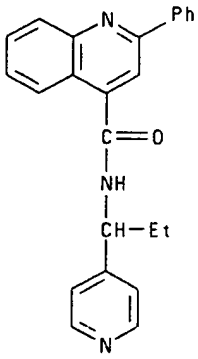
RN 174636-56-7 CA

CN 4-Quinolinecarboxamide, 3-methyl-*N*-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 174636-57-8 CA

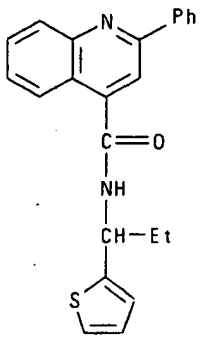
CN 4-Quinolinecarboxamide, 2-phenyl-*N*-[1-(4-pyridinyl)propyl]- (9CI) (CA INDEX NAME)



RN 174636-58-9 CA

CN 4-Quinolinecarboxamide, 2-phenyl-*N*-[1-(2-thienyl)propyl]- (9CI) (CA INDEX NAME)

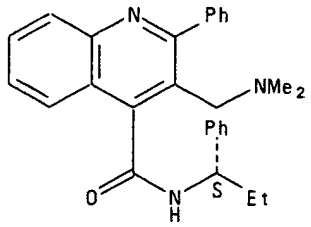
RN 174636-58-9 CA



RN 174636-59-0 CA

CN 4-Quinolinecarboxamide, 3-[(dimethylamino)methyl]-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

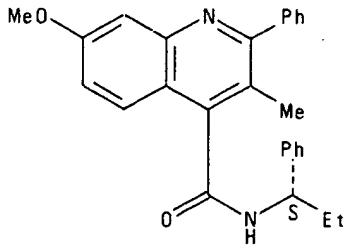
Absolute stereochemistry.



RN 174636-60-3 CA

CN 4-Quinolinecarboxamide, 7-methoxy-3-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

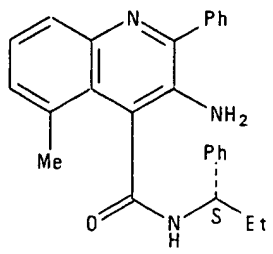


RN 174636-61-4 CA

CN 4-Quinolinecarboxamide, 3-amino-5-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

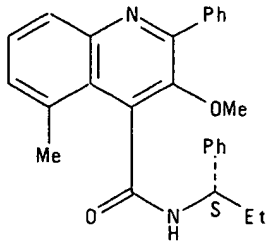
RN 174636-61-4 CA



RN 174636-62-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-5-methyl-2-phenyl-*N*-(1-phenylpropyl)-, (*S*)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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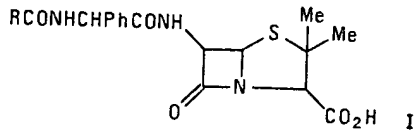
L6 ANSWER 11 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 11
AN 93:186338 CA
TI Ampicillin derivatives
PA Mitsubishi Yuka Yakuhin Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
PI JP 55055194 800422 Showa
AI JP 78-127324 781018
DT Patent
LA Japanese
GI



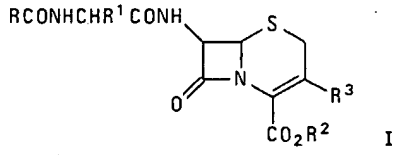
I

AB Fifteen title derivs. I (R = heterocyclic, heterocyclic-substituted methyl) were prepd. and the min. inhibition concns. treated against *Ps. aeruginosa, St. aureus, B. substilis, E. coli, Kl. pneumoniae,* and *Pr. vulgaris.* Thus, 618 mg DCC was added to a mixt. of 648 4-carbamoyl-2-quinolinecarboxylic acid and 345 mg *N*-hydroxysuccinimide in DMF with ice cooling, the mixt. stirred 10 h with ice cooling, a mixt. of 1.2 g ampicillin-$3H_2O$ and 0.42 mL Et_3N in CH_2Cl_2-DMF added, and the mixt. stirred 3 h at room temp. to give, after treating with K 2-ethylhexanoate, 1.32 *d*-I (R = 4-carbamoyl-2-quinolyl) K salt.

IT ***75204-90-9P***
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and bactericidal activity of)

RN 75204-90-9 CA
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[2-(aminocarbonyl)-4-quinolinyl]carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monopotassium salt, [2*S*-[2α,5α,6β(*S**)]]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

L6 ANSWER 12 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 12
AN 90:38949 CA
TI Cephalosporins with α-acylaminoacetic acid side chains
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans
PA Ciba-Geigy A.-G., Switz.
SO Swiss, 11 pp.
CODEN: SWXXAS
PI CH 606006 781013
AI CH 74-6494 740513
DT Patent
LA German
GI



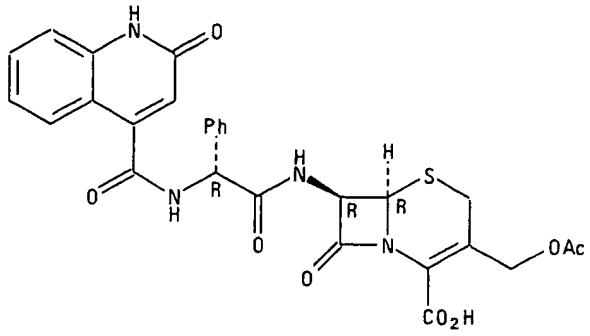
I

AB The cephalosporins I [R = 6-membered ring contg. 1-3 N atoms and an oxo group (optionally substituted or condensed with other rings); R^1 = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R^2 = H, ester group; R^3 = H, alkoxy, substituted Me] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. in mice against *Staphylococcus aureus*. Thus, D-(-)-(1,6-dihydro-6-oxo-3-pyridazinylcarbonylamino)phenylacetic acid reacted with $ClCO_2Et$, *N*-methylmorpholine, and 7β-aminocephalosporanic acid in THF to give D-7β-I (R = 1,6-dihydro-6-oxo-3-pyridazinyl, R^1 = Ph, R^2 = H, R^3 = $AcOCH_2$).

IT ***59133-55-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 59133-55-0 CA
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6*R*-[6α,7β(*R**)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 59133-55-0 CA



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L6 ANSWER 13 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 13

AN 90:38951 CA

TI Cephalosporins with α-acylaminoacetic acid side chains

IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans

PA Ciba-Geigy A.-G., Switz.

SO Swiss, 11 pp.
CODEN: SWXXAS

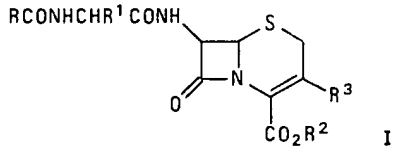
PI CH 606001 781013

AI CH 74-6494 740513

DT Patent

LA German

GI



I

AB The cephemcarboxylic acids I [R = 6-membered ring contg. 1-3 N atoms and an oxo group, optionally substituted or condensed with other rings; R^1 = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R^2 = H, physiol. cleavable ester group; R^3 = H, (substituted) Me, lower alkoxy] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. against *Staphylococcus aureus* in mice. Thus, cephaloglycin reacted with 6-hydroxy-3-pyridinecarbonyl chloride in CH_2Cl_2 to give I (R = 6-hydroxy-3-pyridyl, R^1 = Ph, R^2 = H, R^3 = CH_2OAc).

IT ***59133-55-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 59133-55-0 CA

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6*R*-[6α,7β(*R**)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 14 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 14

AN 84:135637 CA

TI Penicillins

IN Tobiki, Hisao; Shimaji, Kozo; Okano, Shigeru; Komatsu, Toshiaki; Katsura, Toyozo; Taira, Yasushi; Eda, Yasuko

PA Sumitomo Chemical Co., Ltd., Japan

SO Japan., 11 pp.
CODEN: JAXXAD

PI JP 50023036 B4 750805 Showa

AI JP 70-124363 701229

DT Patent

LA Japanese

GI For diagram(s), see printed CA Issue.

AB Acids ROH I (Z = O, S; R1 = alkyl, cycloalkylalkyl, alkenyl, aralkyl, OH, alkoxy, aralkyloxy; R2 = H, alkyl; A = benzo, naphtho, pyrido) were treated with 6-aminopenicillanic acid (III) or its derivs. to give II. II are bactericides not only against gram-pos. and -neg. bacteria but also against Pseudomonas aeruginosa (min. inhibitory concn. 3.13-50 .mu.g/ml). Thus, 2 g 1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxylic acid in CH2Cl2 was treated with Et3N, 1.8 g ClCO2Et, and 1.65 g D(-)-.alpha.-phenylglycine Et ester-HCl to give 1.8 g D(-)-.alpha.-(1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxamido)phenylacetic acid, which (1 g) in CH2Cl2 was treated with Et3N, ClCO2Et and 0.83 g III Et3N salt to give 1.3 g D(-)-II (Z = O, R1 = OH, R2 = H, A = 6,7-methylenedioxybenzo). Among 25 more II prepd. were (Z, R1, R2, A given): O, Et, H, 6-methoxybenzo; O, Me, H, X; O, Et, H, 1,2-naphtho; O, OEt, H, 6,7-methylenedioxybenzo.

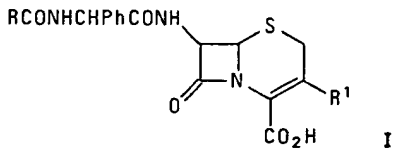
IT ***58865-82-0P***
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and bactericidal activity of)

RN 58865-82-0 CA

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[(3-ethoxy-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2*S*-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 15 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 15
AN 84:164802 CA
TI Cephalosporins with .alpha.-acylaminoacetic acid side chain
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans
PA Ciba-Geigy A.-G., Switz.
SO Ger. Offen., 80 pp.
CODEN: GWXXBX
PI DE 2520561 751127
PRAI CH 74-6494 740513
DT Patent
LA German
GI



I

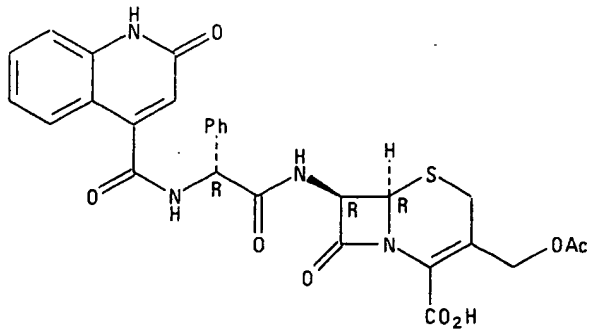
AB Of the cephalosporins I (R = N heterocyclyl, R1 = CH2OAc, OMe, heterocyclic thiomethyl pyridiniomethyl) were prepd. by acetylating cephaloglycines and substituting on acetoxymethyl group. Thus, I (R = 2-hydroxy-5-pyridyl, R1 = OAc) was obtained by treating cephaloglycine with 2-hydroxy-5-pyridinecarbonyl chloride.

IT ***59133-55-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 59133-55-0 CA

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6*R*-[6α,7β(*R**)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 59133-55-0 CA

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L6 ANSWER 16 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 16
AN 70:47439 CA
TI .alpha.-Amidobenzyl- and amido(2-thienyl)methylpenicillins
IN Long, Anthony Alfred W.; Nayler, John H. C.
PA Beecham Group Ltd.
SO Brit., 6 pp.
CODEN: BRXXAA
PI GB 1130445 681016
AI GB 660426
DT Patent
LA English
GI For diagram(s), see printed CA Issue.
AB The 6-aminopenicillanic acid derivs. prepd. had the structure I, where R is a Ph or thienyl group, R1 is a heterocyclic group, and n is 0 or 1. The compds. were useful as antibacterial agents, as nutritional supplements in animal food, and in the treatment of infectious diseases caused by gram-pos. and gram-neg. bacteria. Thus, a suspension of 12.8 g. D-.alpha.-aminobenzylpenicillin (II) trihydrate in 80 ml. H2O was adjusted to pH 9.2 with 5N aq. NaOH and treated with a soln. of 4.6 g. 5-methyl-3-isoxazolecarbonyl chloride in 100 ml. iso-BuCOMe (III). After stirring for 2 hrs. at room temp., the mixt. was filtered through Dicalite and the layers were sepd. The org. phase was washed with satd. brine and treated with 16 ml. 2N Na 2-ethylhexanoate in III to give 13 g. Na salt of D-.alpha.-(5-methyl-3-iso-xazolecarboxamido)benzylpenicillin which crystd. on trituration with ether. The sodium salts of D-.alpha.-(5-methyl-4-isoxazolecar-boxamido)benzylpenicillin, D-.alpha.-(2-furancarboxamido)benzylpenicillin, D-.alpha.-(3-thiophenecarboxamido)benzylpenicillin, D-.alpha.-(2-thiophenecarboxamido)benzylpenicillin, D-.alpha.-(2-thiopheneacetamido)benzylpenicillin, D-.alpha.-(3-thiopheneacetamido)benzylpenicillin, D-.alpha.-(3-ethoxy-4-quinolinecarboxamido)benzylpenicillin, D-.alpha.-(8-methoxy-2-quinolinecarboxamido)benzylpenicillin, D-.alpha.-(2-pyridinecarboxamido)benzylpenicillin, D-.alpha.-(phthalimidoacetamido)-benzylpenicillin, D-.alpha.-(2,6-dioxo-4-piperidineacitamido)benzylpenicillin, D-.alpha.-(2-oxo-2H-pyran-5-carboxamido)benzylpenicillin, D-.alpha.-(5-methyl-3-phenyl-4-isoxazolecarboxamido)benzylpenicillin, D-.alpha.-(3-methyl-5-phenyl-4-isoxazolecarboxamido)benzylpenicillin, D-.alpha.-(5-bromo-2-(methylthio)-4-pyrimidinecarboxamido)benzylpenicillin, D-.alpha.-(2-furoylamino)-2-thienylmethylpenicillin, D-.alpha.-nicotinamidobenzylpenicillin, D-.alpha.-(2-thiopheneacetamido)-2-thi-enylmethylpenicillin, and D-.alpha.-(2-furanacetamido)benzylpenicillin were similarly prepd.
IT ***21611-82-5P***

L6 ANSWER 17 OF 17 CA COPYRIGHT 1997 ACS DUPLICATE 17

AN 74:87972 CA

TI Antibacterial acylated benzylpenicillin and thienylmethylpenicillin derivatives

PA Beecham Group Ltd.

SO Fr. M., 4 pp.
CODEN: FMXXAJ

PI FR 6212 680902

PRAI GB 660426

DT Patent

LA French

GI For diagram(s), see printed CA Issue.

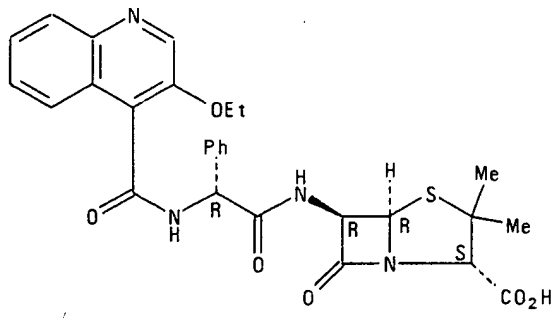
AB [.alpha.-(Amino)arylacetamido]penicillin deriv. (I), where Ar is Ph or 2-thienyl, are treated with Ar1(CH2)nCOCl (Ar1 = heteroaryl) to give penicillin diamide derivs. (II). II (n = 0 or 1 and Ar1 is furyl, thienyl, phthalimido, or a substituted quinolyl, piperidyl, oxopyranyl, or isoxazolyl group) are prepd.

IT ***21611-82-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 21611-82-5 CA

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[2-(3-ethoxycinchoninamido)-2-phenylacetamido]-3,3-dimethyl-7-oxo-, D- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



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